



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 09:44 AM BST

PDB ID : 5GV5  
Title : Crystal structure of *Candida antarctica* Lipase B with active Ser105 modified with a phosphonate inhibitor  
Authors : Park, S.Y.; Lee, H.  
Deposited on : 2016-09-02  
Resolution : 2.89 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

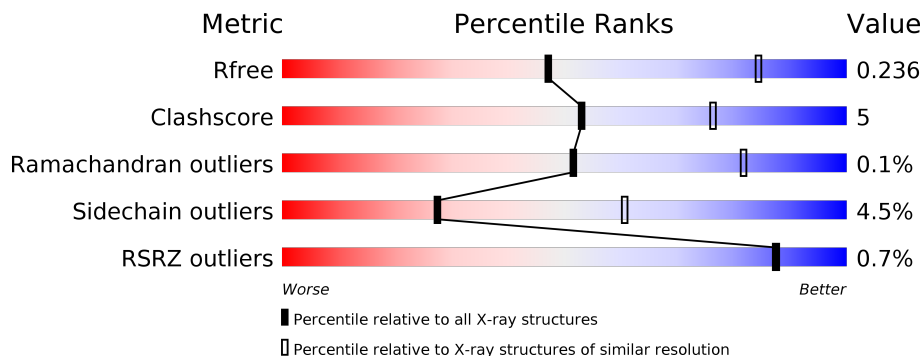
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.89 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	317	86% 13%
1	B	317	86% 14% .
1	C	317	82% 15% .
1	D	317	86% 10% ..
1	E	317	89% 9% ..
1	F	317	85% 14% ..

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Mol	Chain	Length	Quality of chain
1	G	317	 % 86% 14%
1	H	317	 % 83% 15%
2	I	4	 25% 75%
2	K	4	 100%
3	J	2	 100%
3	L	2	 100%
3	M	2	 100%
3	N	2	 100%
3	O	2	 100%
3	P	2	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	K	4	-	-	-	X
3	NAG	M	2	-	-	-	X
3	NAG	N	2	-	-	-	X
3	NAG	O	2	-	-	-	X
3	NAG	P	2	-	-	-	X

## 2 Entry composition i

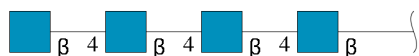
There are 4 unique types of molecules in this entry. The entry contains 18946 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Lipase B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	317	2324	1472	389	453	10	0	0	0
1	B	317	2324	1472	389	453	10	0	0	0
1	C	316	2316	1466	388	452	10	0	0	0
1	D	309	2272	1438	381	443	10	0	0	0
1	E	314	2306	1460	386	450	10	0	0	0
1	F	317	2324	1472	389	453	10	0	0	0
1	G	317	2324	1472	389	453	10	0	0	0
1	H	317	2324	1472	389	453	10	0	0	0

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



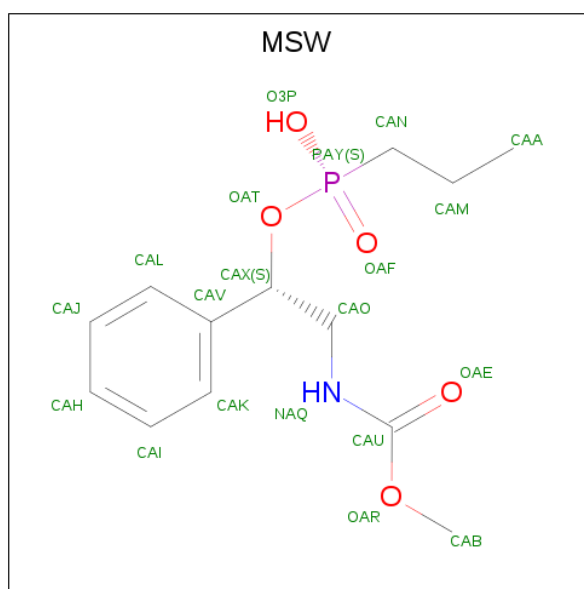
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	I	4	56	32	4	20	0	0	0
2	K	4	56	32	4	20	0	0	0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	P	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is [(1S)-2-(methoxycarbonylamino)-1-phenyl-ethoxy]-propyl-phosphinic acid (three-letter code: MSW) (formula: C<sub>13</sub>H<sub>20</sub>NO<sub>5</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	Total	C	N	O	P	0	0
			19	13	1	4	1		
4	B	1	Total	C	N	O	P	0	0
			19	13	1	4	1		
4	C	1	Total	C	N	O	P	0	0
			19	13	1	4	1		

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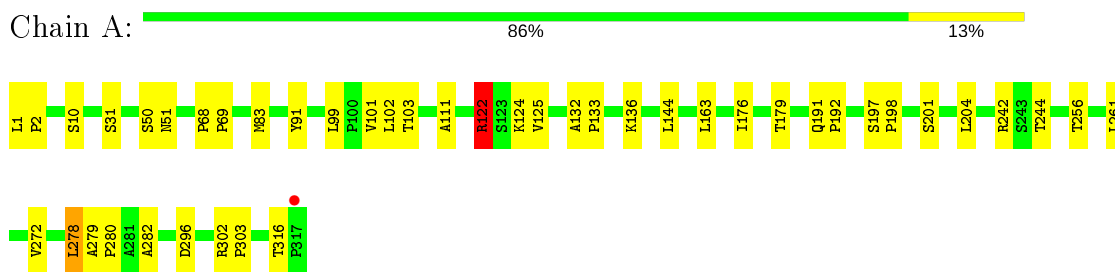
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>					<b>ZeroOcc</b>	<b>AltConf</b>
4	D	1	Total	C	N	O	P	0	0
			19	13	1	4	1		
4	E	1	Total	C	N	O	P	0	0
			19	13	1	4	1		
4	F	1	Total	C	N	O	P	0	0
			19	13	1	4	1		
4	G	1	Total	C	N	O	P	0	0
			19	13	1	4	1		
4	H	1	Total	C	N	O	P	0	0
			19	13	1	4	1		

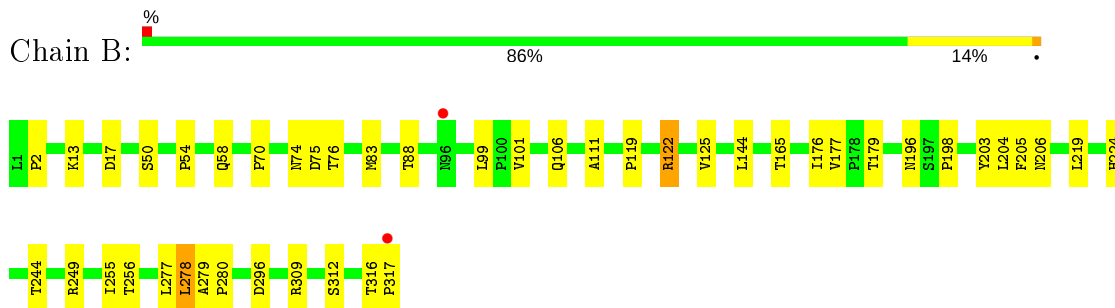
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

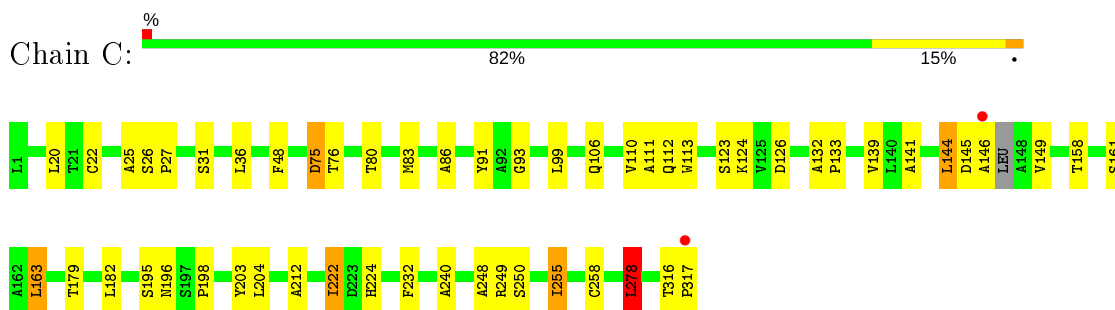
- Molecule 1: Lipase B



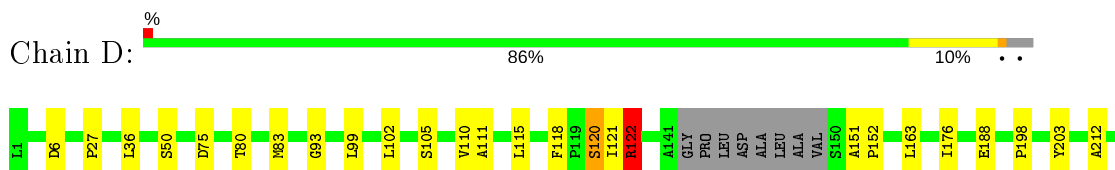
- Molecule 1: Lipase B

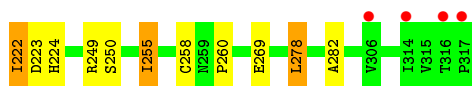


- Molecule 1: Lipase B

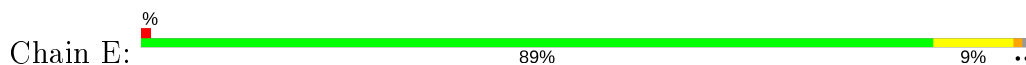


- Molecule 1: Lipase B

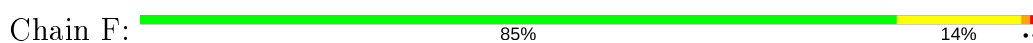




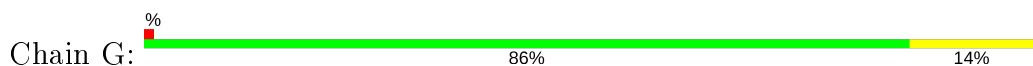
- Molecule 1: Lipase B



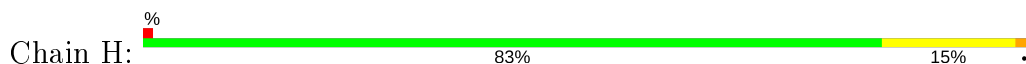
- Molecule 1: Lipase B



- Molecule 1: Lipase B



- Molecule 1: Lipase B



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



Chain I: 25% 75%

MAG1  
MAG2  
MAG3  
MAG4

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 100%

MAG1  
MAG2  
MAG3  
MAG4

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 100%

MAG1  
MAG2

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L: 100%

MAG1  
MAG2

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M: 100%

MAG1  
MAG2

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N: 100%

MAG1  
MAG2

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O: 100%

MAG1  
MAG2

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:

100%

MAG1  
MAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.46Å 123.22Å 150.32Å 90.00° 96.20° 90.00°	Depositor
Resolution (Å)	30.63 – 2.89 30.63 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.2 (30.63-2.89) 99.4 (30.63-2.89)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.29 (at 2.90Å)	Xtrriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.171 , 0.229 0.182 , 0.236	Depositor DCC
$R_{free}$ test set	3753 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.5	Xtrriage
Anisotropy	0.700	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 24.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	18946	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MSW, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.68	0/2383	0.81	4/3272 (0.1%)
1	B	0.64	0/2383	0.79	1/3272 (0.0%)
1	C	0.71	0/2374	0.82	3/3258 (0.1%)
1	D	0.67	0/2329	0.82	2/3195 (0.1%)
1	E	0.68	0/2364	0.79	3/3244 (0.1%)
1	F	0.65	0/2383	0.79	2/3272 (0.1%)
1	G	0.59	0/2383	0.76	1/3272 (0.0%)
1	H	0.59	0/2383	0.75	2/3272 (0.1%)
All	All	0.65	0/18982	0.79	18/26057 (0.1%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	249	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	E	122	ARG	NE-CZ-NH1	7.87	124.24	120.30
1	C	278	LEU	CA-CB-CG	7.19	131.83	115.30
1	F	249	ARG	NE-CZ-NH1	6.73	123.66	120.30
1	A	296	ASP	CB-CG-OD1	6.63	124.27	118.30
1	E	278	LEU	CA-CB-CG	6.30	129.78	115.30
1	H	219	LEU	CB-CG-CD1	-6.02	100.76	111.00
1	F	122	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	296	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	E	105	SER	CB-CA-C	5.57	120.68	110.10
1	A	242	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	C	75	ASP	CB-CG-OD1	5.40	123.16	118.30
1	H	127	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	122	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	D	75	ASP	CB-CG-OD1	5.13	122.91	118.30
1	G	168	ARG	NE-CZ-NH1	5.05	122.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	122	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	B	249	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2324	0	2298	33	0
1	B	2324	0	2297	27	0
1	C	2316	0	2286	32	0
1	D	2272	0	2241	23	0
1	E	2306	0	2276	15	0
1	F	2324	0	2298	27	0
1	G	2324	0	2298	24	0
1	H	2324	0	2298	35	0
2	I	56	0	49	3	0
2	K	56	0	49	0	0
3	J	28	0	25	0	0
3	L	28	0	25	0	0
3	M	28	0	25	0	0
3	N	28	0	25	0	0
3	O	28	0	25	0	0
3	P	28	0	25	0	0
4	A	19	0	0	3	0
4	B	19	0	0	6	0
4	C	19	0	0	4	0
4	D	19	0	0	2	0
4	E	19	0	0	0	0
4	F	19	0	0	1	0
4	G	19	0	0	2	0
4	H	19	0	0	4	0
All	All	18946	0	18540	204	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 5.

All (204) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:278:LEU:CD1	1:D:278:LEU:O	1.98	1.11
1:D:278:LEU:HD13	1:D:278:LEU:O	1.60	0.98
1:F:249:ARG:HG3	1:F:249:ARG:HH11	1.28	0.96
1:D:278:LEU:HD12	1:D:278:LEU:O	1.67	0.92
1:B:278:LEU:HB3	4:B:401:MSW:CAB	2.03	0.88
1:A:10:SER:O	2:I:3:NAG:H61	1.75	0.86
1:A:278:LEU:HD21	1:H:278:LEU:HD11	1.67	0.77
1:C:278:LEU:HB2	4:C:401:MSW:CAB	2.14	0.76
1:D:278:LEU:CD1	1:D:278:LEU:C	2.54	0.76
1:B:278:LEU:HB3	4:B:401:MSW:OAR	1.90	0.72
1:B:224:HIS:HD2	4:B:401:MSW:OAE	1.73	0.71
1:H:40:THR:O	4:H:401:MSW:CAI	2.42	0.67
1:F:182:LEU:HD23	1:F:236:VAL:HG11	1.75	0.67
1:D:278:LEU:HD12	1:D:278:LEU:C	2.15	0.66
1:F:83:MET:SD	1:F:111:ALA:HA	2.37	0.65
1:C:144:LEU:HD22	1:C:144:LEU:N	2.12	0.65
1:A:261:LEU:HD21	1:H:144:LEU:HD22	1.80	0.64
2:I:3:NAG:O6	2:I:4:NAG:N2	2.30	0.64
1:D:278:LEU:CD1	1:D:282:ALA:HB2	2.28	0.63
1:H:83:MET:SD	1:H:111:ALA:HA	2.39	0.63
1:C:144:LEU:HD22	1:C:144:LEU:H	1.64	0.63
1:A:278:LEU:CD2	1:H:278:LEU:HD11	2.28	0.63
1:A:176:ILE:O	1:B:244:THR:OG1	2.16	0.62
1:H:281:ALA:HB1	4:H:401:MSW:CAI	2.29	0.62
1:E:83:MET:SD	1:E:111:ALA:HA	2.39	0.62
1:C:144:LEU:CD2	1:C:144:LEU:H	2.13	0.62
1:C:139:VAL:O	1:C:141:ALA:O	2.18	0.61
1:C:278:LEU:HB2	4:C:401:MSW:OAR	2.00	0.61
1:G:70:PRO:HD2	1:G:74:ASN:HB2	1.83	0.61
1:H:94:SER:O	1:H:97:ASN:ND2	2.35	0.60
1:F:249:ARG:CG	1:F:249:ARG:HH11	2.09	0.60
1:B:2:PRO:O	1:B:122:ARG:NH2	2.29	0.60
1:A:282:ALA:HB1	1:H:275:ALA:HB1	1.82	0.60
1:B:296:ASP:OD2	1:B:312:SER:OG	2.17	0.59
1:A:179:THR:HG21	1:A:204:LEU:HD12	1.85	0.59
1:C:212:ALA:CB	1:C:222:ILE:HD11	2.33	0.59
1:A:272:VAL:HG13	1:H:283:ALA:HB1	1.85	0.58
1:A:83:MET:SD	1:A:111:ALA:HA	2.44	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:THR:HG21	1:C:204:LEU:HD12	1.85	0.58
1:H:224:HIS:CD2	4:H:401:MSW:CAO	2.86	0.58
1:G:102:LEU:HD23	1:G:102:LEU:C	2.24	0.58
1:D:278:LEU:HD11	1:D:282:ALA:HB2	1.85	0.58
1:C:278:LEU:O	1:C:278:LEU:HD22	2.05	0.56
1:F:249:ARG:HG3	1:F:249:ARG:NH1	2.06	0.56
1:C:198:PRO:HA	1:C:203:TYR:CD2	2.39	0.56
1:B:279:ALA:HB3	1:B:280:PRO:HD3	1.87	0.56
1:C:91:TYR:CG	1:C:124:LYS:HG2	2.41	0.56
1:D:198:PRO:HA	1:D:203:TYR:CD1	2.40	0.56
1:H:1:LEU:HD21	1:H:176:ILE:HG12	1.89	0.55
1:F:147:LEU:HB2	1:F:149:VAL:HG13	1.89	0.55
1:D:224:HIS:HD2	4:D:401:MSW:OAE	1.89	0.55
1:A:244:THR:CG2	1:B:176:ILE:O	2.55	0.54
1:F:217:GLY:HA2	1:G:255:ILE:HD12	1.89	0.54
1:A:2:PRO:O	1:A:122:ARG:NH2	2.32	0.54
1:G:83:MET:SD	1:G:111:ALA:HA	2.48	0.54
1:C:255:ILE:HA	1:C:258:CYS:SG	2.48	0.53
1:F:224:HIS:CD2	4:F:401:MSW:OAE	2.62	0.53
1:D:222:ILE:HG23	1:D:260:PRO:HB3	1.89	0.53
1:C:145:ASP:O	1:C:146:ALA:HB3	2.07	0.53
1:H:43:THR:OG1	1:H:45:PRO:HD2	2.09	0.53
1:A:278:LEU:HB2	4:A:401:MSW:OAR	2.09	0.52
1:D:212:ALA:HB3	1:D:222:ILE:HD11	1.92	0.52
1:A:102:LEU:HD23	1:A:102:LEU:C	2.30	0.52
4:B:401:MSW:NAQ	4:B:401:MSW:CAK	2.72	0.52
1:A:279:ALA:HB2	1:H:279:ALA:HB2	1.91	0.52
4:A:401:MSW:CAK	4:A:401:MSW:NAQ	2.73	0.51
1:C:113:TRP:CZ3	1:C:163:LEU:HG	2.46	0.51
1:F:222:ILE:HG23	1:F:260:PRO:HB3	1.93	0.50
1:H:86:ALA:O	1:H:90:LEU:HG	2.10	0.50
1:F:113:TRP:CZ3	1:F:163:LEU:HG	2.47	0.50
1:A:244:THR:HG21	1:B:176:ILE:O	2.13	0.49
1:D:188:GLU:OE1	1:D:223:ASP:HB2	2.13	0.49
1:C:158:THR:O	1:C:161:SER:HB3	2.13	0.48
1:C:144:LEU:N	1:C:144:LEU:CD2	2.73	0.48
1:H:84:VAL:O	1:H:85:ASN:C	2.51	0.48
1:A:244:THR:HG22	1:B:177:VAL:HA	1.95	0.48
1:D:115:LEU:O	1:D:122:ARG:HD3	2.13	0.48
1:C:76:THR:HG23	1:C:106:GLN:OE1	2.13	0.48
1:D:224:HIS:CD2	4:D:401:MSW:OAE	2.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:278:LEU:HB3	4:G:401:MSW:CAB	2.44	0.48
1:A:261:LEU:HD12	1:H:147:LEU:HD13	1.94	0.47
1:A:272:VAL:HG13	1:H:283:ALA:CB	2.44	0.47
1:C:83:MET:SD	1:C:111:ALA:HA	2.55	0.47
2:I:2:NAG:H61	2:I:3:NAG:O5	2.14	0.47
1:F:6:ASP:OD2	1:F:120:SER:OG	2.18	0.47
1:F:279:ALA:N	1:F:280:PRO:HD2	2.29	0.47
1:B:205:PHE:O	1:B:206:ASN:HB2	2.16	0.46
1:E:7:PRO:HG2	1:E:300:TYR:CD2	2.50	0.46
1:C:112:GLN:HA	1:C:112:GLN:OE1	2.14	0.46
1:B:277:LEU:O	1:B:280:PRO:HD2	2.15	0.46
1:B:224:HIS:CD2	4:B:401:MSW:OAE	2.61	0.46
1:A:191:GLN:OE1	1:A:192:PRO:HA	2.16	0.46
1:C:22:CYS:HB2	1:C:25:ALA:O	2.15	0.46
1:H:279:ALA:HB3	1:H:280:PRO:HD3	1.98	0.46
1:E:179:THR:HG21	1:E:204:LEU:HD12	1.97	0.46
1:B:76:THR:HG23	1:B:106:GLN:OE1	2.16	0.45
1:E:119:PRO:HA	1:E:122:ARG:HG3	1.98	0.45
1:F:195:SER:HG	1:F:197:SER:HG	1.58	0.45
1:F:136:LYS:HE2	1:F:200:ASP:O	2.17	0.45
1:B:83:MET:SD	1:B:111:ALA:HA	2.57	0.45
1:D:255:ILE:HA	1:D:258:CYS:SG	2.56	0.45
1:H:37:VAL:HG13	1:H:66:ILE:HD11	1.98	0.45
1:H:115:LEU:O	1:H:122:ARG:HD3	2.15	0.45
1:H:197:SER:HB2	1:H:198:PRO:HD2	1.99	0.45
1:C:316:THR:O	1:C:317:PRO:C	2.55	0.45
1:H:316:THR:HB	1:H:317:PRO:CD	2.46	0.45
1:C:27:PRO:O	1:C:93:GLY:HA3	2.17	0.45
1:E:2:PRO:O	1:E:122:ARG:NH2	2.44	0.45
1:B:278:LEU:HD13	1:G:278:LEU:HD21	1.98	0.45
1:D:83:MET:SD	1:D:111:ALA:HA	2.58	0.44
1:B:278:LEU:HD13	1:G:278:LEU:CD2	2.47	0.44
1:A:144:LEU:HD22	1:H:261:LEU:HD21	1.98	0.44
1:G:152:PRO:O	1:G:156:GLN:HG3	2.18	0.44
1:H:240:ALA:HB2	1:H:248:ALA:HB2	1.99	0.44
1:B:101:VAL:HG23	1:B:125:VAL:HG13	2.00	0.44
1:F:148:ALA:HB1	1:F:292:ASN:HB3	1.98	0.44
1:E:149:VAL:HG12	1:E:290:LYS:HB3	1.98	0.44
1:E:184:SER:HB2	1:E:222:ILE:CG2	2.47	0.44
1:B:119:PRO:HA	1:B:122:ARG:HG3	2.00	0.44
1:B:54:PRO:O	1:B:58:GLN:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:182:LEU:HD21	1:E:232:PHE:CE2	2.53	0.44
1:D:122:ARG:HD2	1:D:176:ILE:CG2	2.47	0.44
1:A:91:TYR:CD2	1:A:124:LYS:HE2	2.53	0.43
1:C:91:TYR:CD1	1:C:124:LYS:HG2	2.53	0.43
1:A:101:VAL:HG23	1:A:125:VAL:HG13	2.01	0.43
1:H:36:LEU:HA	1:H:102:LEU:O	2.18	0.43
1:A:102:LEU:HD23	1:A:103:THR:N	2.33	0.43
4:C:401:MSW:CAK	4:C:401:MSW:NAQ	2.81	0.43
1:G:37:VAL:HG13	1:G:66:ILE:HD11	1.98	0.43
1:H:222:ILE:HD12	1:H:227:SER:HA	2.00	0.43
1:G:119:PRO:HA	1:G:122:ARG:HG3	2.01	0.43
1:G:12:PRO:HB2	1:G:15:VAL:HG23	2.00	0.43
1:G:222:ILE:HD12	1:G:227:SER:HA	2.00	0.43
1:G:278:LEU:HD13	1:G:278:LEU:H	1.83	0.43
1:H:51:ASN:OD1	1:H:52:TRP:HD1	2.00	0.43
1:C:198:PRO:HG3	1:C:203:TYR:CE2	2.53	0.43
1:E:115:LEU:O	1:E:122:ARG:HD3	2.19	0.43
1:B:316:THR:HB	1:B:317:PRO:HD2	2.01	0.43
1:C:195:SER:O	1:C:196:ASN:C	2.57	0.43
1:E:139:VAL:O	1:E:141:ALA:O	2.37	0.43
1:C:36:LEU:HB3	1:C:48:PHE:CE2	2.54	0.43
1:H:51:ASN:O	1:H:55:LEU:HG	2.19	0.43
1:A:144:LEU:N	1:A:144:LEU:HD23	2.33	0.43
1:D:27:PRO:O	1:D:93:GLY:HA3	2.19	0.42
1:E:255:ILE:HA	1:E:258:CYS:SG	2.59	0.42
1:H:197:SER:CB	1:H:198:PRO:CD	2.97	0.42
1:F:224:HIS:O	1:F:227:SER:HB2	2.19	0.42
1:D:80:THR:HA	1:D:110:VAL:HG13	2.02	0.42
1:F:195:SER:OG	1:F:197:SER:OG	2.32	0.42
1:B:179:THR:HG21	1:B:204:LEU:HD12	2.01	0.42
1:F:68:PRO:HA	1:F:69:PRO:HD3	1.93	0.42
1:A:279:ALA:HB3	1:A:280:PRO:HD3	2.01	0.42
1:F:261:LEU:HB3	1:F:262:PRO:CD	2.50	0.42
1:G:119:PRO:O	1:G:122:ARG:HG3	2.19	0.42
1:G:27:PRO:O	1:G:93:GLY:HA3	2.19	0.42
1:G:80:THR:HA	1:G:110:VAL:HG13	2.00	0.42
1:A:132:ALA:N	1:A:133:PRO:CD	2.82	0.42
1:B:70:PRO:HD2	1:B:74:ASN:HB2	2.01	0.42
1:G:44:GLY:N	1:G:45:PRO:CD	2.83	0.42
1:A:244:THR:CG2	1:B:177:VAL:HG12	2.50	0.42
1:E:271:LYS:HB2	1:H:199:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:119:PRO:O	1:F:122:ARG:HG3	2.19	0.42
1:G:52:TRP:HA	1:G:55:LEU:HB2	2.01	0.42
1:G:132:ALA:N	1:G:133:PRO:CD	2.83	0.42
1:E:113:TRP:CZ3	1:E:163:LEU:HG	2.55	0.41
1:F:174:THR:HG22	1:F:175:GLN:O	2.19	0.41
1:A:68:PRO:HA	1:A:69:PRO:HD3	1.96	0.41
1:B:278:LEU:CB	4:B:401:MSW:CAB	2.88	0.41
1:D:118:PHE:O	1:D:121:ILE:HG12	2.20	0.41
1:F:141:ALA:HA	1:F:144:LEU:HD12	2.02	0.41
1:H:238:ARG:O	1:H:239:SER:C	2.58	0.41
1:A:197:SER:HB2	1:A:198:PRO:CD	2.50	0.41
1:C:132:ALA:N	1:C:133:PRO:CD	2.83	0.41
4:G:401:MSW:CAK	4:G:401:MSW:NAQ	2.84	0.41
1:C:182:LEU:HD21	1:C:232:PHE:CE2	2.55	0.41
1:C:240:ALA:HB2	1:C:248:ALA:HB2	2.03	0.41
1:D:151:ALA:O	1:D:152:PRO:C	2.59	0.41
1:F:106:GLN:HG2	1:F:110:VAL:HG23	2.03	0.41
1:C:80:THR:HA	1:C:110:VAL:HG13	2.02	0.41
1:C:20:LEU:HD13	1:C:86:ALA:HB1	2.02	0.41
1:E:238:ARG:HD2	1:E:242:ARG:HH21	1.85	0.41
1:D:6:ASP:OD1	1:D:120:SER:HB3	2.20	0.41
1:F:255:ILE:HD12	1:F:256:THR:H	1.85	0.41
1:F:302:ARG:N	1:F:303:PRO:HD2	2.36	0.41
1:A:278:LEU:HA	4:A:401:MSW:OAE	2.20	0.41
1:E:119:PRO:O	1:E:122:ARG:HG3	2.21	0.41
1:H:119:PRO:O	1:H:122:ARG:HG3	2.19	0.41
1:A:136:LYS:HG3	1:A:201:SER:HA	2.02	0.41
1:F:227:SER:O	1:F:233:SER:OG	2.29	0.41
1:G:1:LEU:HD12	1:G:1:LEU:HA	1.87	0.41
1:B:13:LYS:O	1:B:17:ASP:OD2	2.39	0.41
1:G:112:GLN:OE1	1:G:112:GLN:HA	2.20	0.41
1:H:40:THR:O	4:H:401:MSW:CAK	2.69	0.41
1:C:224:HIS:CD2	4:C:401:MSW:OAE	2.74	0.40
1:D:36:LEU:HD23	1:D:102:LEU:HB3	2.03	0.40
1:G:24:GLY:O	1:G:25:ALA:HB2	2.22	0.40
1:H:306:VAL:HG13	1:H:316:THR:HA	2.04	0.40
1:A:1:LEU:HD12	1:A:1:LEU:HA	1.91	0.40
1:A:302:ARG:N	1:A:303:PRO:CD	2.85	0.40
1:B:198:PRO:HA	1:B:203:TYR:CG	2.57	0.40
1:F:148:ALA:CB	1:F:292:ASN:HB3	2.52	0.40
1:G:184:SER:HB2	1:G:222:ILE:HG13	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:316:THR:HB	1:G:317:PRO:HD2	2.03	0.40
1:H:278:LEU:CD1	1:H:279:ALA:N	2.84	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	315/317 (99%)	301 (96%)	14 (4%)	0	100	100
1	B	315/317 (99%)	302 (96%)	13 (4%)	0	100	100
1	C	312/317 (98%)	287 (92%)	25 (8%)	0	100	100
1	D	305/317 (96%)	284 (93%)	21 (7%)	0	100	100
1	E	310/317 (98%)	296 (96%)	14 (4%)	0	100	100
1	F	315/317 (99%)	292 (93%)	23 (7%)	0	100	100
1	G	315/317 (99%)	295 (94%)	20 (6%)	0	100	100
1	H	315/317 (99%)	292 (93%)	21 (7%)	2 (1%)	25	58
All	All	2502/2536 (99%)	2349 (94%)	151 (6%)	2 (0%)	51	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	93	GLY
1	H	281	ALA

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	255/255 (100%)	246 (96%)	9 (4%)	36	70
1	B	255/255 (100%)	242 (95%)	13 (5%)	24	56
1	C	254/255 (100%)	241 (95%)	13 (5%)	24	56
1	D	250/255 (98%)	238 (95%)	12 (5%)	25	58
1	E	254/255 (100%)	245 (96%)	9 (4%)	36	70
1	F	255/255 (100%)	243 (95%)	12 (5%)	26	59
1	G	255/255 (100%)	243 (95%)	12 (5%)	26	59
1	H	255/255 (100%)	243 (95%)	12 (5%)	26	59
All	All	2033/2040 (100%)	1941 (96%)	92 (4%)	27	61

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	SER
1	A	50	SER
1	A	51	ASN
1	A	99	LEU
1	A	122	ARG
1	A	163	LEU
1	A	256	THR
1	A	278	LEU
1	A	316	THR
1	B	50	SER
1	B	75	ASP
1	B	88	THR
1	B	99	LEU
1	B	122	ARG
1	B	144	LEU
1	B	165	THR
1	B	196	ASN
1	B	219	LEU
1	B	255	ILE
1	B	256	THR
1	B	278	LEU
1	B	309	ARG
1	C	26	SER
1	C	31	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	75	ASP
1	C	99	LEU
1	C	123	SER
1	C	126	ASP
1	C	144	LEU
1	C	149	VAL
1	C	163	LEU
1	C	222	ILE
1	C	250	SER
1	C	255	ILE
1	C	278	LEU
1	D	50	SER
1	D	99	LEU
1	D	105	SER
1	D	120	SER
1	D	122	ARG
1	D	163	LEU
1	D	222	ILE
1	D	249	ARG
1	D	250	SER
1	D	255	ILE
1	D	269	GLU
1	D	278	LEU
1	E	32	LYS
1	E	50	SER
1	E	51	ASN
1	E	99	LEU
1	E	123	SER
1	E	126	ASP
1	E	182	LEU
1	E	255	ILE
1	E	278	LEU
1	F	28	SER
1	F	32	LYS
1	F	99	LEU
1	F	122	ARG
1	F	138	THR
1	F	184	SER
1	F	186	THR
1	F	195	SER
1	F	222	ILE
1	F	249	ARG

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Mol	Chain	Res	Type
1	F	250	SER
1	F	255	ILE
1	G	5	SER
1	G	50	SER
1	G	51	ASN
1	G	83	MET
1	G	99	LEU
1	G	138	THR
1	G	144	LEU
1	G	195	SER
1	G	196	ASN
1	G	256	THR
1	G	278	LEU
1	G	302	ARG
1	H	1	LEU
1	H	32	LYS
1	H	50	SER
1	H	51	ASN
1	H	122	ARG
1	H	143	PRO
1	H	144	LEU
1	H	249	ARG
1	H	256	THR
1	H	269	GLU
1	H	278	LEU
1	H	306	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	196	ASN
1	C	264	ASN
1	D	196	ASN
1	D	224	HIS
1	E	196	ASN
1	F	196	ASN
1	G	196	ASN
1	H	51	ASN
1	H	196	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

20 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	J	2	3	14,14,15	0.64	0	17,19,21	1.44	4 (23%)
3	NAG	L	2	3	14,14,15	0.79	0	17,19,21	1.57	3 (17%)
2	NAG	K	2	2	14,14,15	0.69	0	17,19,21	2.52	6 (35%)
3	NAG	N	2	3	14,14,15	0.62	0	17,19,21	1.15	1 (5%)
2	NAG	K	4	2	14,14,15	0.74	0	17,19,21	2.18	6 (35%)
2	NAG	I	3	2	14,14,15	1.04	0	17,19,21	2.17	5 (29%)
2	NAG	K	3	2	14,14,15	1.08	1 (7%)	17,19,21	2.28	5 (29%)
3	NAG	O	2	3	14,14,15	0.76	0	17,19,21	2.99	7 (41%)
3	NAG	P	2	3	14,14,15	0.59	0	17,19,21	1.28	3 (17%)
2	NAG	I	2	2	14,14,15	0.74	1 (7%)	17,19,21	2.70	7 (41%)
3	NAG	M	2	3	14,14,15	0.75	0	17,19,21	1.71	5 (29%)
2	NAG	K	1	1,2	14,14,15	0.79	0	17,19,21	1.46	5 (29%)
3	NAG	L	1	1,3	14,14,15	0.79	1 (7%)	17,19,21	1.66	3 (17%)
2	NAG	I	1	1,2	14,14,15	0.85	0	17,19,21	1.48	4 (23%)
3	NAG	J	1	1,3	14,14,15	0.89	1 (7%)	17,19,21	1.51	3 (17%)
3	NAG	O	1	1,3	14,14,15	0.82	0	17,19,21	1.88	7 (41%)
3	NAG	P	1	1,3	14,14,15	0.62	0	17,19,21	1.28	2 (11%)
3	NAG	M	1	1,3	14,14,15	0.86	1 (7%)	17,19,21	1.77	5 (29%)
3	NAG	N	1	1,3	14,14,15	0.76	0	17,19,21	1.38	2 (11%)
2	NAG	I	4	2	14,14,15	0.51	0	17,19,21	1.53	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	J	2	3	-	1/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
3	NAG	N	2	3	-	0/6/23/26	0/1/1/1
2	NAG	K	4	2	-	2/6/23/26	0/1/1/1
2	NAG	I	3	2	-	2/6/23/26	0/1/1/1
2	NAG	K	3	2	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	4/6/23/26	0/1/1/1
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	1/6/23/26	0/1/1/1
3	NAG	L	1	1,3	-	2/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	O	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	P	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	M	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	N	1	1,3	-	1/6/23/26	0/1/1/1
2	NAG	I	4	2	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	1	NAG	O5-C1	-2.60	1.39	1.43
2	K	3	NAG	C1-C2	2.41	1.55	1.52
2	I	2	NAG	O5-C1	-2.39	1.39	1.43
3	M	1	NAG	O5-C1	-2.30	1.40	1.43
3	L	1	NAG	O5-C1	-2.20	1.40	1.43

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	2	NAG	C1-O5-C5	8.20	123.31	112.19
2	I	2	NAG	O4-C4-C3	-7.59	92.81	110.35
2	K	2	NAG	O4-C4-C5	6.04	124.29	109.30
2	K	4	NAG	C1-O5-C5	5.78	120.03	112.19
2	K	2	NAG	O4-C4-C3	-5.19	98.35	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	3	NAG	C1-C2-N2	4.98	118.99	110.49
2	I	3	NAG	C4-C3-C2	4.81	118.07	111.02
3	O	2	NAG	C8-C7-N2	4.75	124.15	116.10
2	I	4	NAG	O5-C5-C6	4.07	113.58	107.20
2	I	3	NAG	O6-C6-C5	4.01	125.05	111.29
2	K	2	NAG	C1-O5-C5	4.01	117.62	112.19
2	K	3	NAG	C4-C3-C2	3.91	116.74	111.02
2	I	2	NAG	C1-O5-C5	3.89	117.46	112.19
2	K	3	NAG	C2-N2-C7	3.77	128.27	122.90
3	L	2	NAG	O5-C5-C6	3.70	113.01	107.20
2	I	3	NAG	C2-N2-C7	3.69	128.16	122.90
3	O	1	NAG	C1-O5-C5	3.62	117.10	112.19
2	I	2	NAG	O4-C4-C5	3.57	118.16	109.30
2	K	4	NAG	O5-C1-C2	3.44	116.72	111.29
2	I	4	NAG	C4-C3-C2	3.39	115.98	111.02
3	O	2	NAG	O5-C5-C6	3.36	112.47	107.20
3	J	1	NAG	O5-C5-C4	-3.31	102.78	110.83
3	L	1	NAG	C3-C4-C5	-3.28	104.39	110.24
3	M	2	NAG	C1-C2-N2	3.18	115.91	110.49
3	M	1	NAG	O3-C3-C2	-3.14	102.97	109.47
3	M	1	NAG	C1-C2-N2	-3.13	105.14	110.49
3	L	1	NAG	O4-C4-C3	-3.12	103.13	110.35
2	I	2	NAG	O5-C1-C2	-3.07	106.44	111.29
2	I	3	NAG	O5-C5-C4	-3.06	103.37	110.83
3	L	1	NAG	O5-C1-C2	-3.06	106.46	111.29
3	O	2	NAG	O5-C5-C4	3.03	118.20	110.83
3	J	2	NAG	C4-C3-C2	3.00	115.42	111.02
2	I	2	NAG	C4-C3-C2	2.99	115.41	111.02
3	O	2	NAG	C4-C3-C2	-2.99	106.63	111.02
2	K	3	NAG	O7-C7-C8	-2.99	116.51	122.06
2	K	3	NAG	O5-C5-C6	2.98	111.88	107.20
3	J	2	NAG	O5-C5-C4	-2.95	103.65	110.83
3	O	2	NAG	O5-C1-C2	-2.92	106.68	111.29
3	M	2	NAG	O5-C5-C6	2.91	111.76	107.20
3	O	1	NAG	C6-C5-C4	2.88	119.76	113.00
3	N	1	NAG	C1-O5-C5	2.88	116.09	112.19
3	O	2	NAG	O7-C7-C8	-2.86	116.74	122.06
3	M	2	NAG	C4-C3-C2	2.85	115.20	111.02
2	I	2	NAG	O5-C5-C6	-2.82	102.78	107.20
2	K	2	NAG	C1-C2-N2	2.66	115.03	110.49
2	K	1	NAG	O3-C3-C2	-2.62	104.05	109.47
2	I	1	NAG	O5-C1-C2	-2.61	107.16	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	2	NAG	O5-C5-C4	-2.60	104.50	110.83
2	K	4	NAG	O7-C7-C8	-2.60	117.24	122.06
3	P	1	NAG	C1-O5-C5	2.57	115.67	112.19
3	M	1	NAG	C4-C3-C2	2.57	114.78	111.02
3	P	2	NAG	O5-C5-C6	2.56	111.22	107.20
2	K	4	NAG	C4-C3-C2	2.49	114.67	111.02
3	P	1	NAG	C4-C3-C2	2.49	114.66	111.02
2	I	3	NAG	C6-C5-C4	2.48	118.81	113.00
2	I	1	NAG	O6-C6-C5	-2.45	102.89	111.29
3	J	1	NAG	C4-C3-C2	2.42	114.57	111.02
2	K	2	NAG	C4-C3-C2	2.40	114.53	111.02
3	M	2	NAG	C3-C4-C5	-2.37	106.00	110.24
2	I	1	NAG	O7-C7-N2	2.37	126.31	121.95
3	N	1	NAG	C3-C4-C5	-2.37	106.01	110.24
3	O	1	NAG	O7-C7-C8	-2.36	117.68	122.06
3	O	1	NAG	O4-C4-C5	2.34	115.12	109.30
3	M	1	NAG	O5-C5-C6	-2.34	103.53	107.20
3	L	2	NAG	O5-C5-C4	-2.31	105.21	110.83
2	K	4	NAG	O5-C5-C6	2.29	110.80	107.20
2	K	1	NAG	C4-C3-C2	2.29	114.38	111.02
2	I	1	NAG	C8-C7-N2	-2.28	112.23	116.10
2	I	2	NAG	C3-C4-C5	-2.25	106.23	110.24
3	O	1	NAG	C8-C7-N2	2.21	119.85	116.10
3	P	2	NAG	O7-C7-C8	-2.21	117.96	122.06
2	K	1	NAG	O4-C4-C3	-2.20	105.27	110.35
2	K	1	NAG	C6-C5-C4	2.19	118.13	113.00
3	J	2	NAG	O5-C5-C6	2.14	110.56	107.20
3	O	1	NAG	C3-C4-C5	-2.14	106.43	110.24
3	M	1	NAG	O7-C7-N2	2.12	125.84	121.95
3	J	2	NAG	O7-C7-C8	-2.09	118.18	122.06
3	N	2	NAG	O7-C7-C8	-2.09	118.18	122.06
2	K	1	NAG	O7-C7-N2	2.08	125.77	121.95
3	J	1	NAG	O4-C4-C5	2.08	114.45	109.30
3	P	2	NAG	C1-O5-C5	2.07	114.99	112.19
3	O	1	NAG	O6-C6-C5	2.05	118.32	111.29
3	L	2	NAG	C3-C4-C5	-2.02	106.64	110.24
2	K	4	NAG	C3-C4-C5	-2.01	106.64	110.24
2	K	2	NAG	C8-C7-N2	2.01	119.50	116.10

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	2	NAG	O5-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
2	I	3	NAG	O5-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
3	O	2	NAG	C4-C5-C6-O6
2	K	4	NAG	C4-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
3	O	2	NAG	C8-C7-N2-C2
3	O	2	NAG	O7-C7-N2-C2
2	I	2	NAG	C4-C5-C6-O6
2	K	4	NAG	O5-C5-C6-O6
2	I	3	NAG	C4-C5-C6-O6
2	I	4	NAG	C4-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
2	K	1	NAG	C4-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
3	N	1	NAG	O5-C5-C6-O6
2	I	4	NAG	O5-C5-C6-O6
3	M	2	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	3	NAG	3	0
2	I	2	NAG	1	0
2	I	4	NAG	1	0

## 5.5 Carbohydrates [i](#)

20 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	I	1	1,2	14,14,15	0.85	0	17,19,21	1.48	4 (23%)
2	NAG	I	2	2	14,14,15	0.74	1 (7%)	17,19,21	2.70	7 (41%)
2	NAG	I	3	2	14,14,15	1.04	0	17,19,21	2.17	5 (29%)
2	NAG	I	4	2	14,14,15	0.51	0	17,19,21	1.53	2 (11%)
3	NAG	J	1	1,3	14,14,15	0.89	1 (7%)	17,19,21	1.51	3 (17%)
3	NAG	J	2	3	14,14,15	0.64	0	17,19,21	1.44	4 (23%)
2	NAG	K	1	1,2	14,14,15	0.79	0	17,19,21	1.46	5 (29%)
2	NAG	K	2	2	14,14,15	0.69	0	17,19,21	2.52	6 (35%)
2	NAG	K	3	2	14,14,15	1.08	1 (7%)	17,19,21	2.28	5 (29%)
2	NAG	K	4	2	14,14,15	0.74	0	17,19,21	2.18	6 (35%)
3	NAG	L	1	1,3	14,14,15	0.79	1 (7%)	17,19,21	1.66	3 (17%)
3	NAG	L	2	3	14,14,15	0.79	0	17,19,21	1.57	3 (17%)
3	NAG	M	1	1,3	14,14,15	0.86	1 (7%)	17,19,21	1.77	5 (29%)
3	NAG	M	2	3	14,14,15	0.75	0	17,19,21	1.71	5 (29%)
3	NAG	N	1	1,3	14,14,15	0.76	0	17,19,21	1.38	2 (11%)
3	NAG	N	2	3	14,14,15	0.62	0	17,19,21	1.15	1 (5%)
3	NAG	O	1	1,3	14,14,15	0.82	0	17,19,21	1.88	7 (41%)
3	NAG	O	2	3	14,14,15	0.76	0	17,19,21	2.99	7 (41%)
3	NAG	P	1	1,3	14,14,15	0.62	0	17,19,21	1.28	2 (11%)
3	NAG	P	2	3	14,14,15	0.59	0	17,19,21	1.28	3 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	3	2	-	2/6/23/26	0/1/1/1
2	NAG	I	4	2	-	2/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	1/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	3	2	-	0/6/23/26	0/1/1/1
2	NAG	K	4	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	L	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
3	NAG	M	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
3	NAG	N	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	N	2	3	-	0/6/23/26	0/1/1/1
3	NAG	O	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	4/6/23/26	0/1/1/1
3	NAG	P	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	1	NAG	O5-C1	-2.60	1.39	1.43
2	K	3	NAG	C1-C2	2.41	1.55	1.52
2	I	2	NAG	O5-C1	-2.39	1.39	1.43
3	M	1	NAG	O5-C1	-2.30	1.40	1.43
3	L	1	NAG	O5-C1	-2.20	1.40	1.43

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	2	NAG	C1-O5-C5	8.20	123.31	112.19
2	I	2	NAG	O4-C4-C3	-7.59	92.81	110.35
2	K	2	NAG	O4-C4-C5	6.04	124.29	109.30
2	K	4	NAG	C1-O5-C5	5.78	120.03	112.19
2	K	2	NAG	O4-C4-C3	-5.19	98.35	110.35
2	K	3	NAG	C1-C2-N2	4.98	118.99	110.49
2	I	3	NAG	C4-C3-C2	4.81	118.07	111.02
3	O	2	NAG	C8-C7-N2	4.75	124.15	116.10
2	I	4	NAG	O5-C5-C6	4.07	113.58	107.20
2	I	3	NAG	O6-C6-C5	4.01	125.05	111.29
2	K	2	NAG	C1-O5-C5	4.01	117.62	112.19
2	K	3	NAG	C4-C3-C2	3.91	116.74	111.02
2	I	2	NAG	C1-O5-C5	3.89	117.46	112.19
2	K	3	NAG	C2-N2-C7	3.77	128.27	122.90
3	L	2	NAG	O5-C5-C6	3.70	113.01	107.20
2	I	3	NAG	C2-N2-C7	3.69	128.16	122.90
3	O	1	NAG	C1-O5-C5	3.62	117.10	112.19
2	I	2	NAG	O4-C4-C5	3.57	118.16	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	4	NAG	O5-C1-C2	3.44	116.72	111.29
2	I	4	NAG	C4-C3-C2	3.39	115.98	111.02
3	O	2	NAG	O5-C5-C6	3.36	112.47	107.20
3	J	1	NAG	O5-C5-C4	-3.31	102.78	110.83
3	L	1	NAG	C3-C4-C5	-3.28	104.39	110.24
3	M	2	NAG	C1-C2-N2	3.18	115.91	110.49
3	M	1	NAG	O3-C3-C2	-3.14	102.97	109.47
3	M	1	NAG	C1-C2-N2	-3.13	105.14	110.49
3	L	1	NAG	O4-C4-C3	-3.12	103.13	110.35
2	I	2	NAG	O5-C1-C2	-3.07	106.44	111.29
2	I	3	NAG	O5-C5-C4	-3.06	103.37	110.83
3	L	1	NAG	O5-C1-C2	-3.06	106.46	111.29
3	O	2	NAG	O5-C5-C4	3.03	118.20	110.83
3	J	2	NAG	C4-C3-C2	3.00	115.42	111.02
2	I	2	NAG	C4-C3-C2	2.99	115.41	111.02
3	O	2	NAG	C4-C3-C2	-2.99	106.63	111.02
2	K	3	NAG	O7-C7-C8	-2.99	116.51	122.06
2	K	3	NAG	O5-C5-C6	2.98	111.88	107.20
3	J	2	NAG	O5-C5-C4	-2.95	103.65	110.83
3	O	2	NAG	O5-C1-C2	-2.92	106.68	111.29
3	M	2	NAG	O5-C5-C6	2.91	111.76	107.20
3	O	1	NAG	C6-C5-C4	2.88	119.76	113.00
3	N	1	NAG	C1-O5-C5	2.88	116.09	112.19
3	O	2	NAG	O7-C7-C8	-2.86	116.74	122.06
3	M	2	NAG	C4-C3-C2	2.85	115.20	111.02
2	I	2	NAG	O5-C5-C6	-2.82	102.78	107.20
2	K	2	NAG	C1-C2-N2	2.66	115.03	110.49
2	K	1	NAG	O3-C3-C2	-2.62	104.05	109.47
2	I	1	NAG	O5-C1-C2	-2.61	107.16	111.29
3	M	2	NAG	O5-C5-C4	-2.60	104.50	110.83
2	K	4	NAG	O7-C7-C8	-2.60	117.24	122.06
3	P	1	NAG	C1-O5-C5	2.57	115.67	112.19
3	M	1	NAG	C4-C3-C2	2.57	114.78	111.02
3	P	2	NAG	O5-C5-C6	2.56	111.22	107.20
2	K	4	NAG	C4-C3-C2	2.49	114.67	111.02
3	P	1	NAG	C4-C3-C2	2.49	114.66	111.02
2	I	3	NAG	C6-C5-C4	2.48	118.81	113.00
2	I	1	NAG	O6-C6-C5	-2.45	102.89	111.29
3	J	1	NAG	C4-C3-C2	2.42	114.57	111.02
2	K	2	NAG	C4-C3-C2	2.40	114.53	111.02
3	M	2	NAG	C3-C4-C5	-2.37	106.00	110.24
2	I	1	NAG	O7-C7-N2	2.37	126.31	121.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	1	NAG	C3-C4-C5	-2.37	106.01	110.24
3	O	1	NAG	O7-C7-C8	-2.36	117.68	122.06
3	O	1	NAG	O4-C4-C5	2.34	115.12	109.30
3	M	1	NAG	O5-C5-C6	-2.34	103.53	107.20
3	L	2	NAG	O5-C5-C4	-2.31	105.21	110.83
2	K	4	NAG	O5-C5-C6	2.29	110.80	107.20
2	K	1	NAG	C4-C3-C2	2.29	114.38	111.02
2	I	1	NAG	C8-C7-N2	-2.28	112.23	116.10
2	I	2	NAG	C3-C4-C5	-2.25	106.23	110.24
3	O	1	NAG	C8-C7-N2	2.21	119.85	116.10
3	P	2	NAG	O7-C7-C8	-2.21	117.96	122.06
2	K	1	NAG	O4-C4-C3	-2.20	105.27	110.35
2	K	1	NAG	C6-C5-C4	2.19	118.13	113.00
3	J	2	NAG	O5-C5-C6	2.14	110.56	107.20
3	O	1	NAG	C3-C4-C5	-2.14	106.43	110.24
3	M	1	NAG	O7-C7-N2	2.12	125.84	121.95
3	J	2	NAG	O7-C7-C8	-2.09	118.18	122.06
3	N	2	NAG	O7-C7-C8	-2.09	118.18	122.06
2	K	1	NAG	O7-C7-N2	2.08	125.77	121.95
3	J	1	NAG	O4-C4-C5	2.08	114.45	109.30
3	P	2	NAG	C1-O5-C5	2.07	114.99	112.19
3	O	1	NAG	O6-C6-C5	2.05	118.32	111.29
3	L	2	NAG	C3-C4-C5	-2.02	106.64	110.24
2	K	4	NAG	C3-C4-C5	-2.01	106.64	110.24
2	K	2	NAG	C8-C7-N2	2.01	119.50	116.10

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	2	NAG	O5-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
2	I	3	NAG	O5-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
3	O	2	NAG	C4-C5-C6-O6
2	K	4	NAG	C4-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
3	O	2	NAG	C8-C7-N2-C2
3	O	2	NAG	O7-C7-N2-C2
2	I	2	NAG	C4-C5-C6-O6

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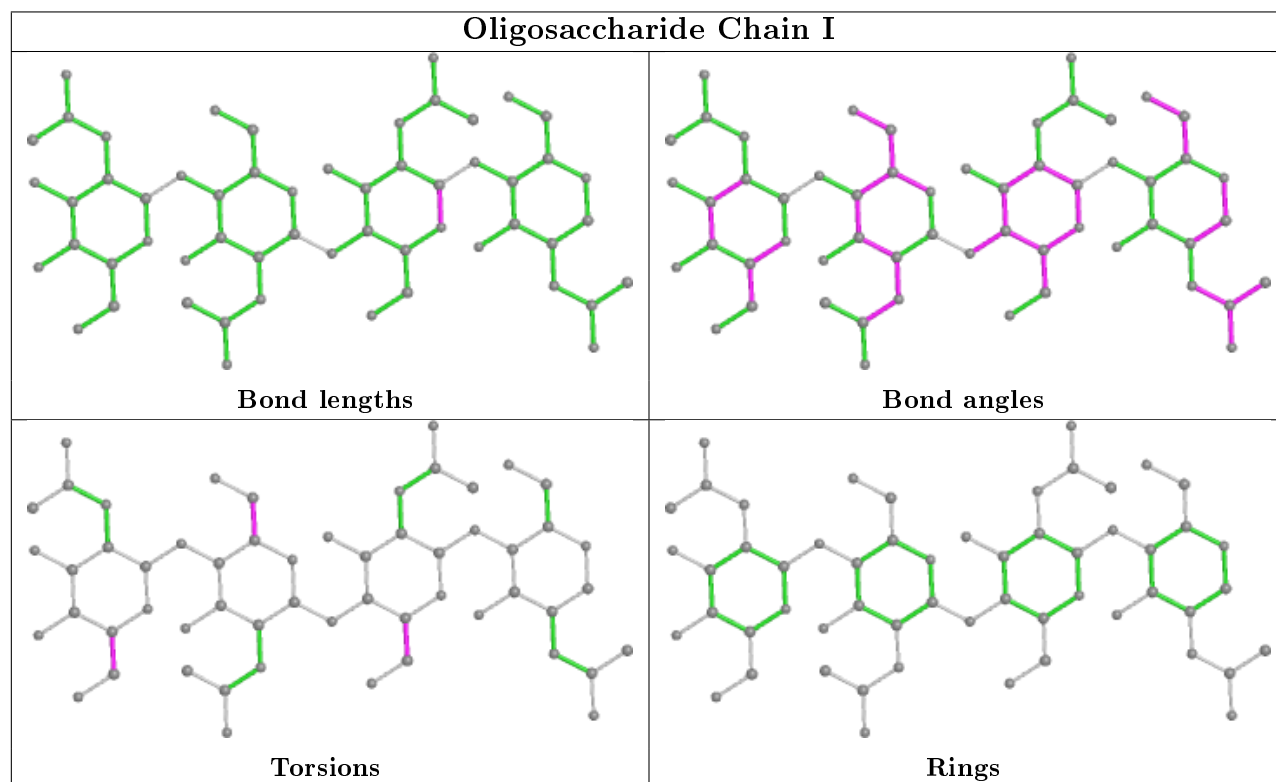
Mol	Chain	Res	Type	Atoms
2	K	4	NAG	O5-C5-C6-O6
2	I	3	NAG	C4-C5-C6-O6
2	I	4	NAG	C4-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
2	K	1	NAG	C4-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
3	N	1	NAG	O5-C5-C6-O6
2	I	4	NAG	O5-C5-C6-O6
3	M	2	NAG	C4-C5-C6-O6

There are no ring outliers.

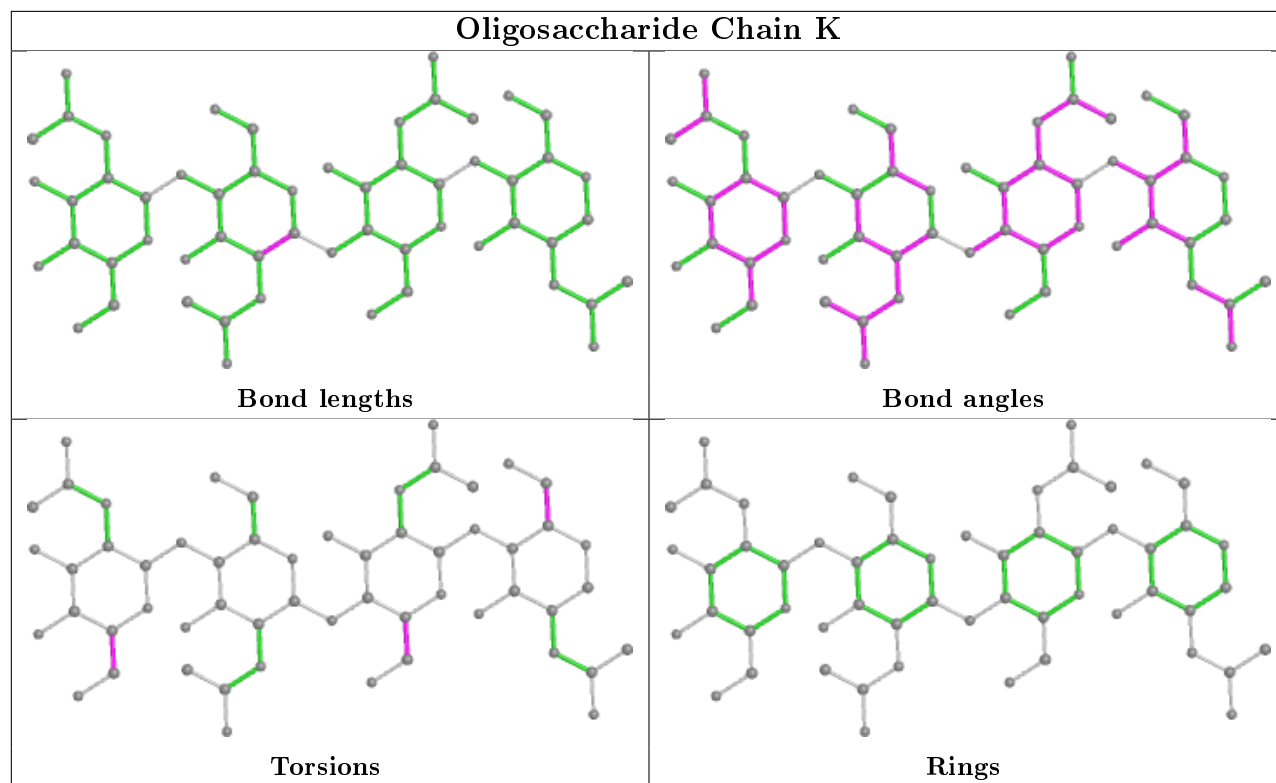
3 monomers are involved in 3 short contacts:

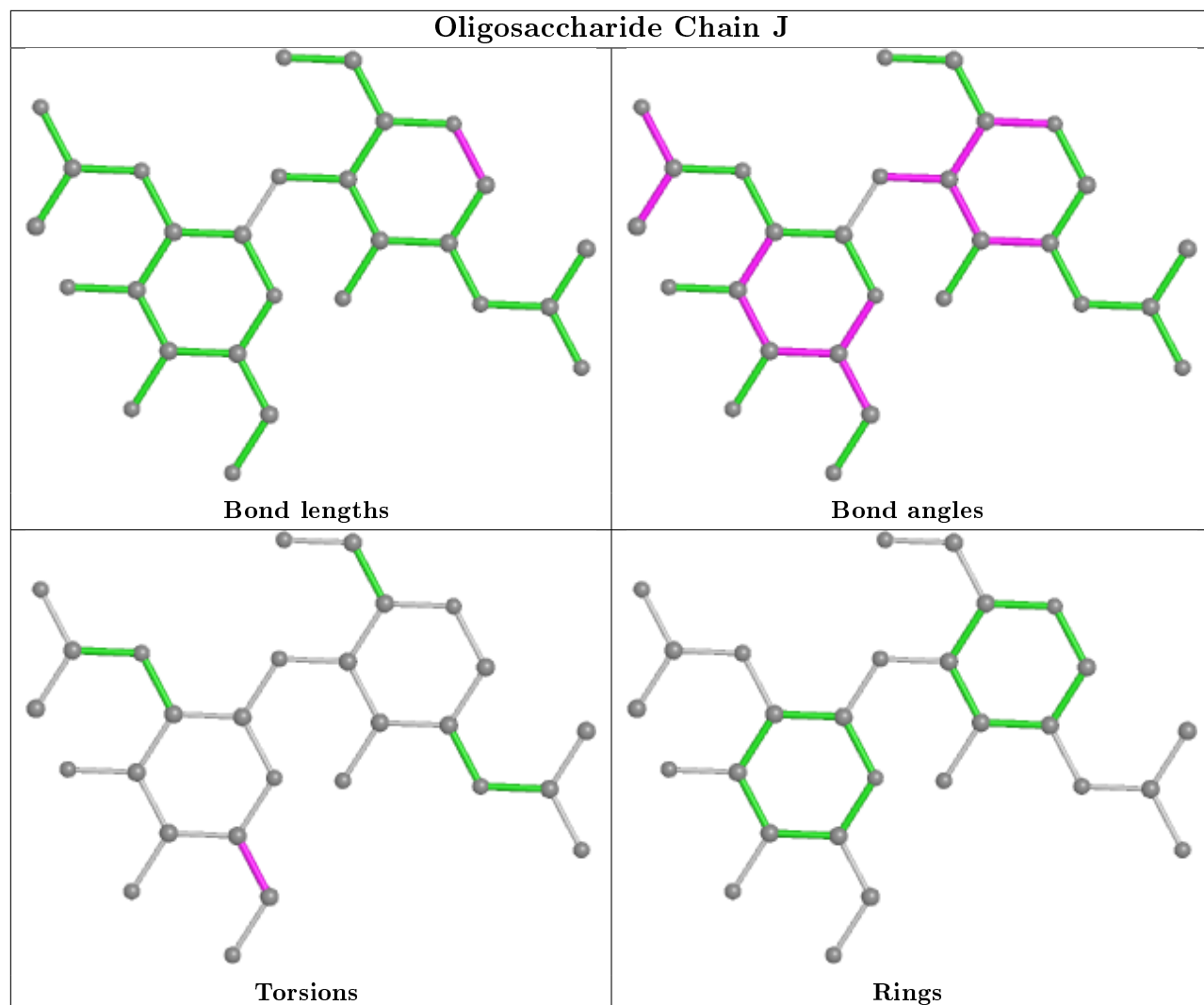
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	3	NAG	3	0
2	I	2	NAG	1	0
2	I	4	NAG	1	0

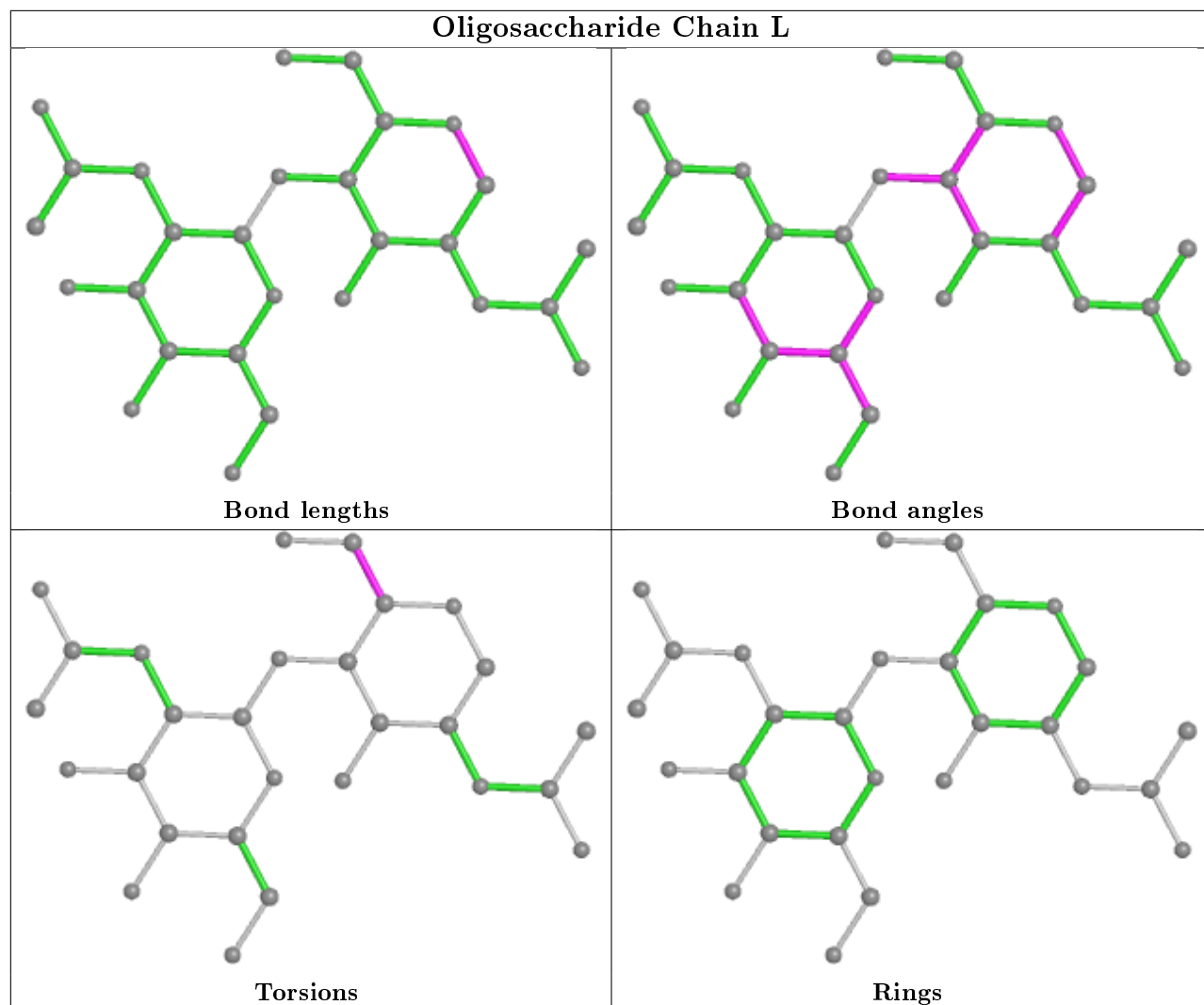
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

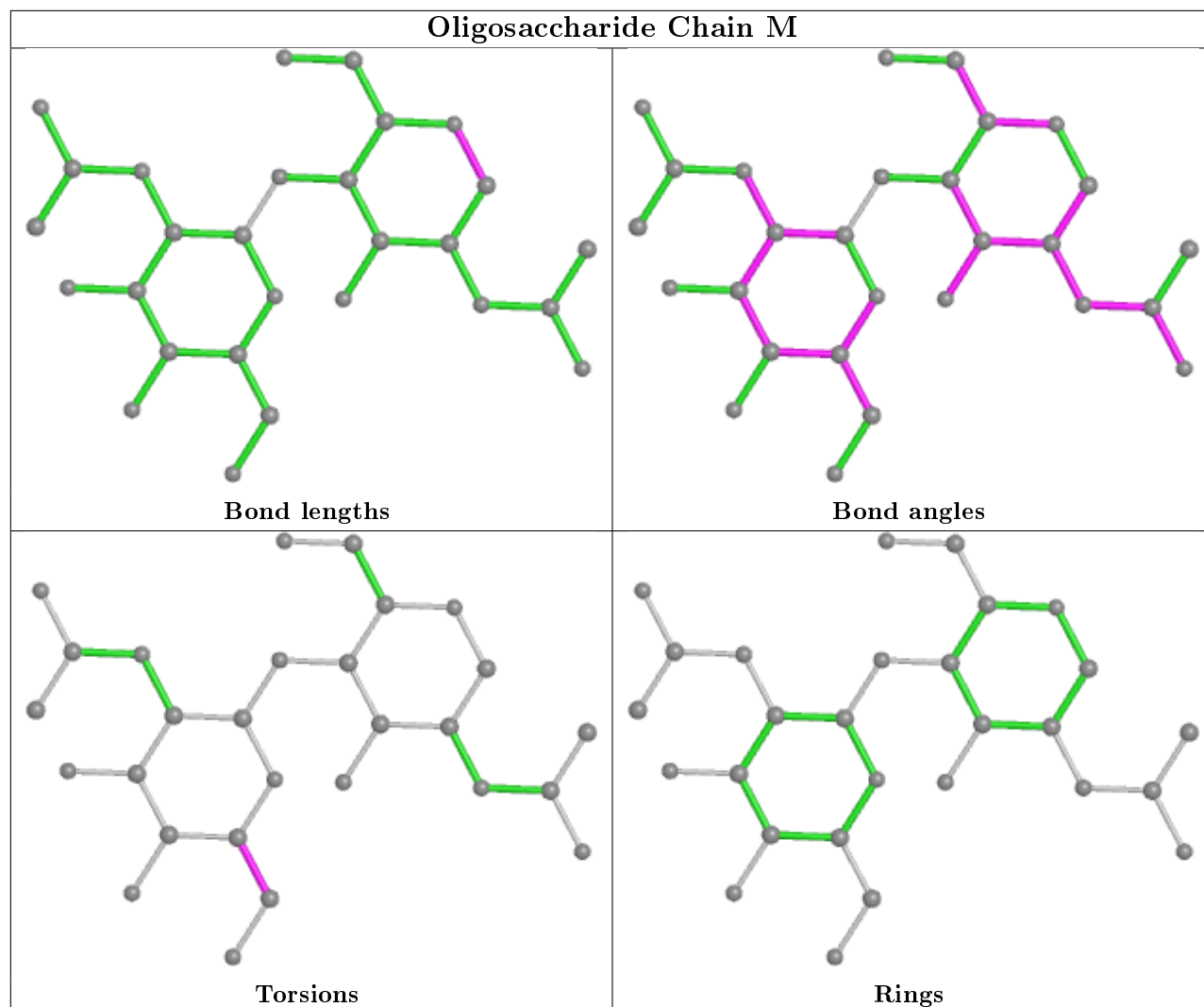


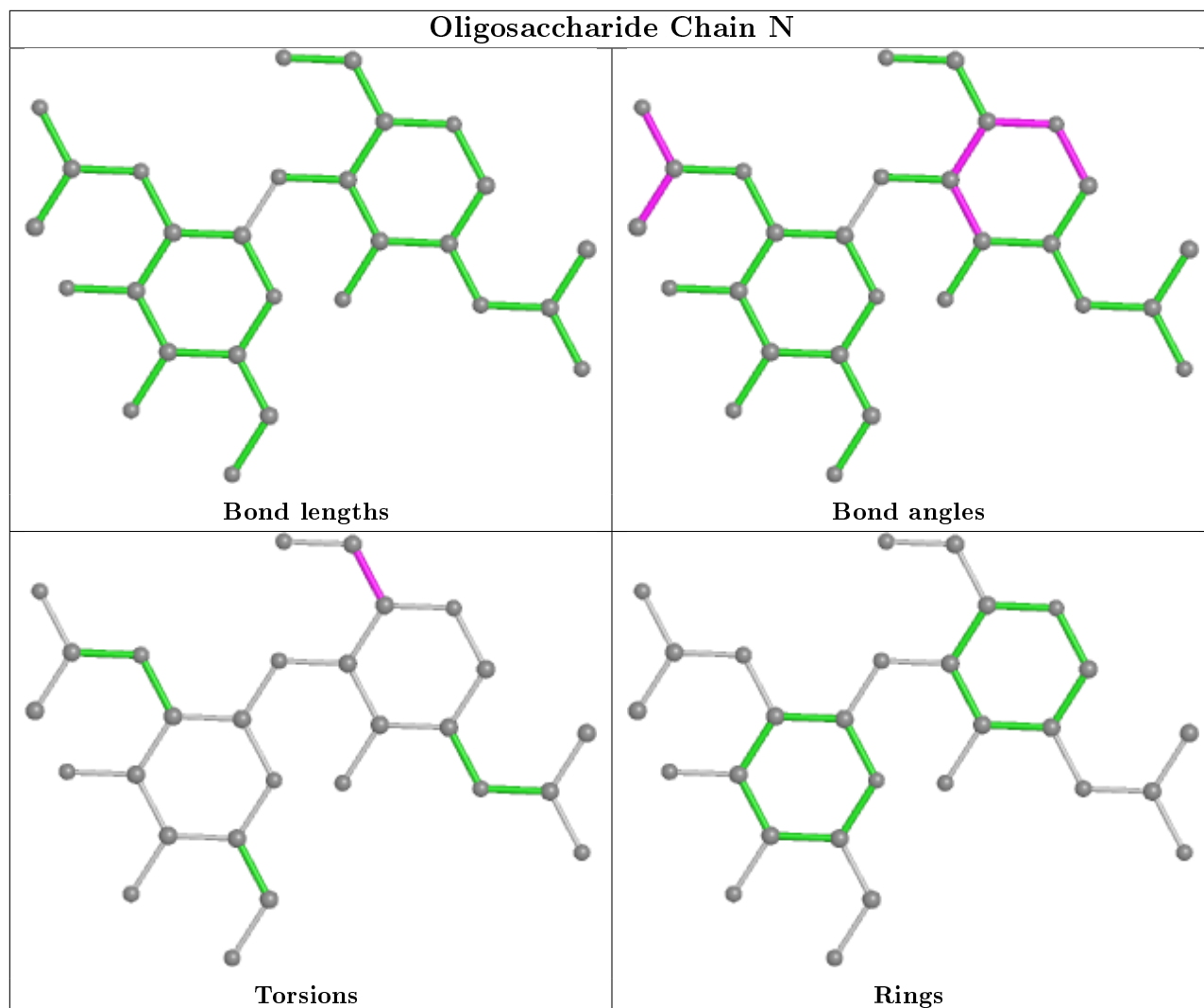


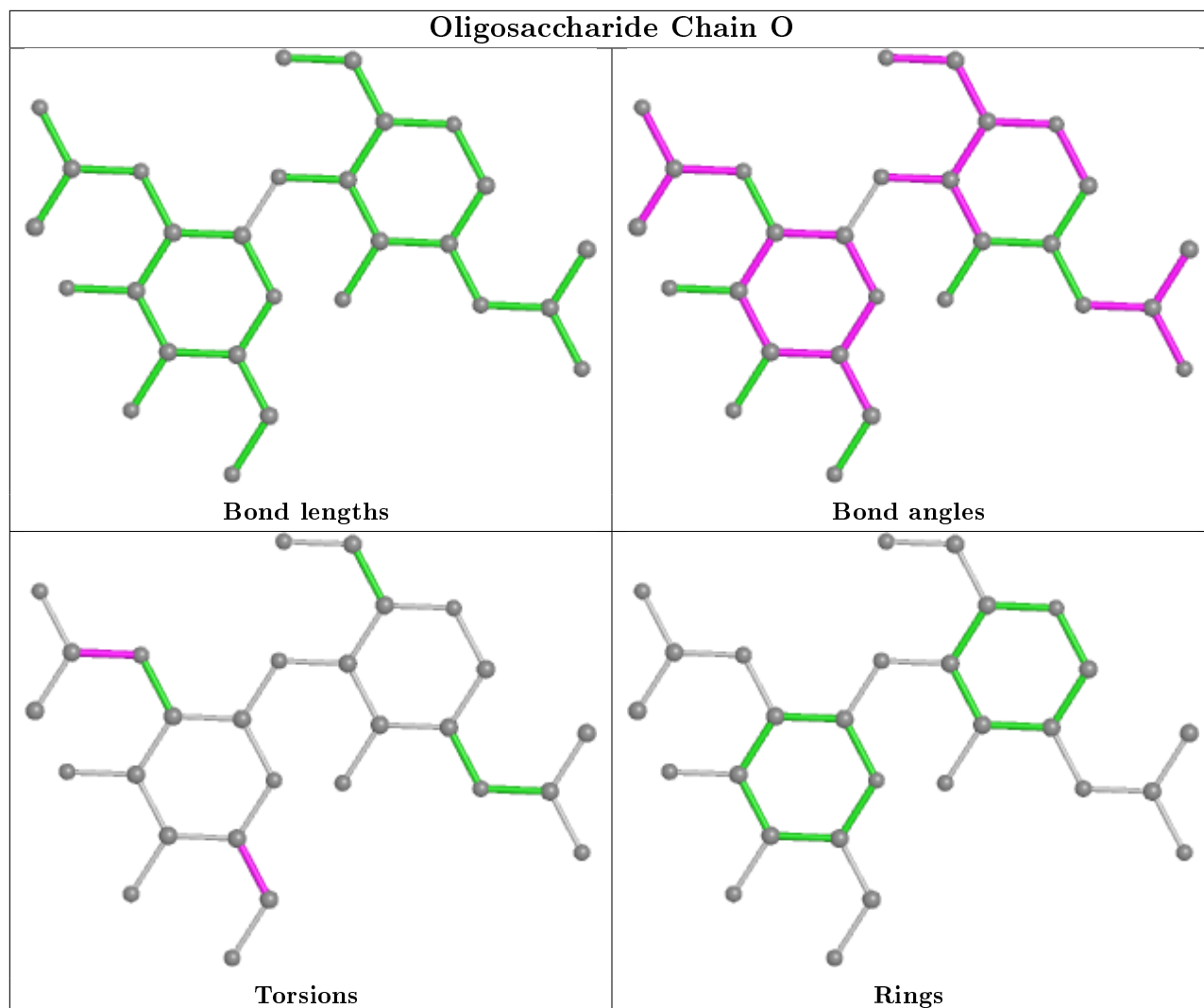


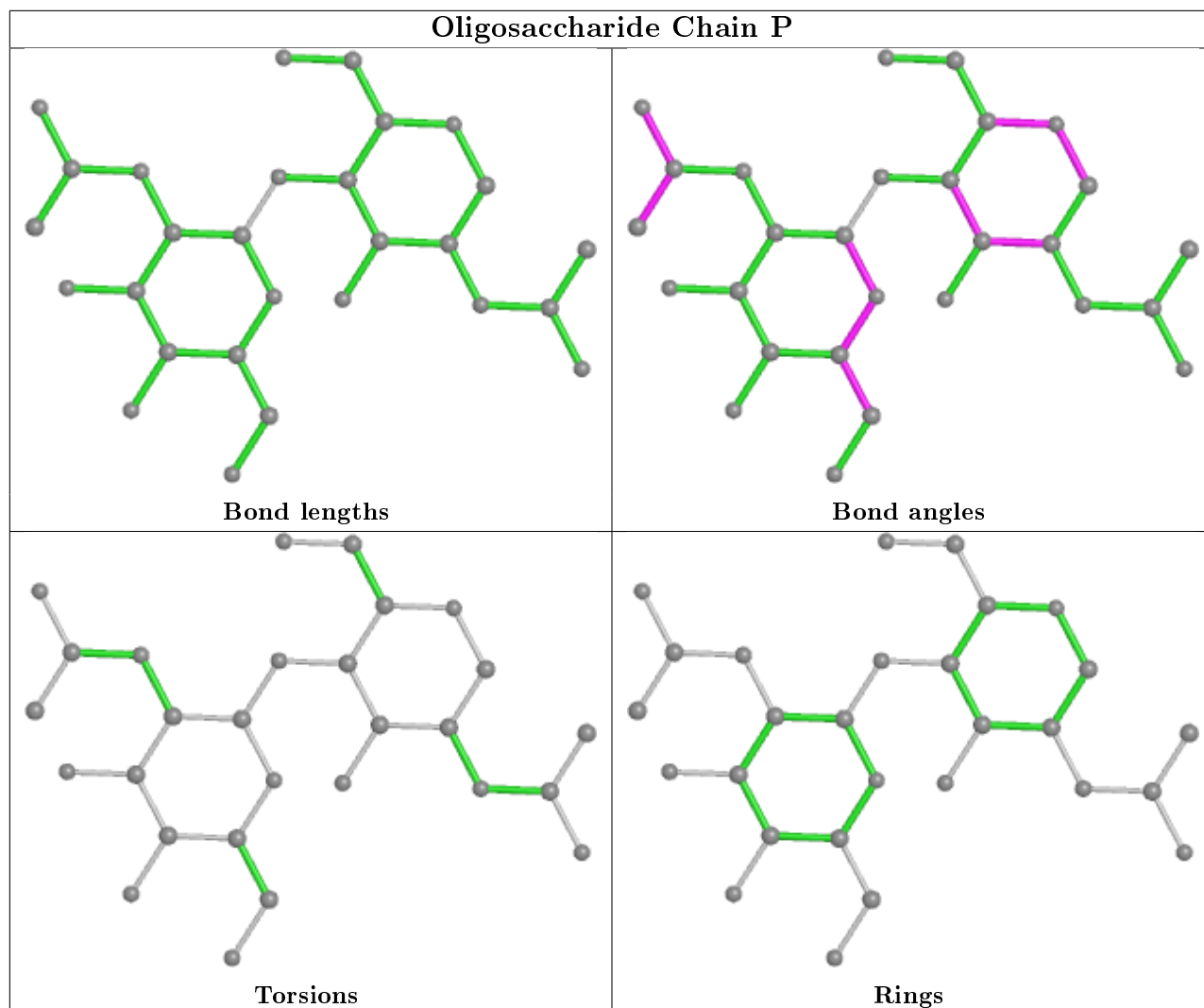












## 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	MSW	C	401	1	15,19,20	1.66	4 (26%)	18,23,26	3.91	10 (55%)
4	MSW	B	401	1	15,19,20	1.55	3 (20%)	18,23,26	4.13	11 (61%)
4	MSW	E	401	1	15,19,20	1.86	4 (26%)	18,23,26	3.52	10 (55%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MSW	D	401	1	15,19,20	0.98	1 (6%)	18,23,26	3.15	5 (27%)
4	MSW	G	401	1	15,19,20	2.42	6 (40%)	18,23,26	4.03	8 (44%)
4	MSW	H	401	1	15,19,20	2.85	2 (13%)	18,23,26	3.16	9 (50%)
4	MSW	F	401	1	15,19,20	1.96	4 (26%)	18,23,26	3.69	5 (27%)
4	MSW	A	401	1	15,19,20	2.22	6 (40%)	18,23,26	3.99	11 (61%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MSW	C	401	1	-	6/12/18/20	0/1/1/1
4	MSW	B	401	1	-	6/12/18/20	0/1/1/1
4	MSW	E	401	1	-	4/12/18/20	0/1/1/1
4	MSW	D	401	1	-	4/12/18/20	0/1/1/1
4	MSW	G	401	1	-	7/12/18/20	0/1/1/1
4	MSW	H	401	1	-	4/12/18/20	0/1/1/1
4	MSW	F	401	1	-	4/12/18/20	0/1/1/1
4	MSW	A	401	1	-	7/12/18/20	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	401	MSW	CAV-CAX	-9.98	1.34	1.51
4	F	401	MSW	CAM-CAN	-4.94	1.48	1.53
4	G	401	MSW	CAV-CAX	4.67	1.59	1.51
4	G	401	MSW	CAK-CAV	4.21	1.45	1.39
4	A	401	MSW	CAV-CAX	4.21	1.58	1.51
4	E	401	MSW	OAR-CAU	3.96	1.41	1.34
4	A	401	MSW	CAK-CAV	3.66	1.45	1.39
4	G	401	MSW	CAL-CAV	3.64	1.44	1.39
4	G	401	MSW	OAR-CAU	3.62	1.40	1.34
4	F	401	MSW	CAV-CAX	-3.60	1.45	1.51
4	A	401	MSW	CAL-CAV	3.53	1.44	1.39
4	H	401	MSW	CAM-CAN	3.10	1.56	1.53
4	E	401	MSW	CAM-CAN	-3.02	1.50	1.53
4	C	401	MSW	OAR-CAU	2.87	1.39	1.34
4	B	401	MSW	CAK-CAV	2.80	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	401	MSW	CAM-CAN	-2.57	1.50	1.53
4	C	401	MSW	CAO-CAX	2.56	1.59	1.51
4	A	401	MSW	CAJ-CAL	2.35	1.43	1.38
4	B	401	MSW	CAO-CAX	2.32	1.58	1.51
4	G	401	MSW	CAO-NAQ	2.26	1.52	1.46
4	E	401	MSW	CAU-NAQ	2.25	1.39	1.34
4	F	401	MSW	CAO-NAQ	2.25	1.52	1.46
4	B	401	MSW	OAR-CAU	2.21	1.38	1.34
4	E	401	MSW	CAK-CAV	2.20	1.42	1.39
4	A	401	MSW	CAI-CAK	2.13	1.43	1.38
4	D	401	MSW	CAV-CAX	-2.11	1.47	1.51
4	A	401	MSW	CAM-CAN	-2.10	1.51	1.53
4	C	401	MSW	CAO-NAQ	2.04	1.52	1.46
4	G	401	MSW	CAU-NAQ	2.02	1.38	1.34
4	F	401	MSW	CAU-NAQ	2.02	1.38	1.34

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	401	MSW	OAR-CAU-NAQ	12.45	124.38	110.93
4	C	401	MSW	OAR-CAU-NAQ	12.40	124.32	110.93
4	B	401	MSW	OAR-CAU-NAQ	11.27	123.10	110.93
4	G	401	MSW	OAR-CAU-NAQ	10.61	122.39	110.93
4	D	401	MSW	OAR-CAU-NAQ	9.34	121.02	110.93
4	E	401	MSW	OAR-CAU-NAQ	9.00	120.65	110.93
4	A	401	MSW	OAR-CAU-NAQ	8.90	120.54	110.93
4	A	401	MSW	OAT-CAX-CAV	8.11	123.86	109.32
4	G	401	MSW	OAT-CAX-CAV	8.03	123.73	109.32
4	H	401	MSW	OAR-CAU-NAQ	7.50	119.03	110.93
4	A	401	MSW	CAL-CAV-CAK	-6.49	110.20	118.29
4	H	401	MSW	CAO-CAX-CAV	-6.35	101.33	111.36
4	F	401	MSW	OAR-CAU-OAE	-6.08	115.64	124.58
4	B	401	MSW	CAL-CAV-CAK	-5.96	110.86	118.29
4	G	401	MSW	CAL-CAV-CAK	-5.71	111.17	118.29
4	E	401	MSW	OAT-CAX-CAO	5.60	113.86	106.22
4	D	401	MSW	CAB-OAR-CAU	-5.53	109.13	115.66
4	D	401	MSW	OAR-CAU-OAE	-5.42	116.61	124.58
4	B	401	MSW	CAO-CAX-CAV	5.01	119.28	111.36
4	E	401	MSW	CAB-OAR-CAU	4.92	121.47	115.66
4	B	401	MSW	OAR-CAU-OAE	-4.89	117.39	124.58
4	E	401	MSW	OAT-CAX-CAV	4.82	117.96	109.32
4	B	401	MSW	CAI-CAK-CAV	4.81	126.60	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	401	MSW	CAB-OAR-CAU	-4.73	110.08	115.66
4	C	401	MSW	OAE-CAU-NAQ	-4.62	117.88	124.96
4	C	401	MSW	OAR-CAU-OAE	-4.61	117.80	124.58
4	A	401	MSW	CAJ-CAL-CAV	4.45	126.15	120.65
4	E	401	MSW	CAO-NAQ-CAU	4.44	128.19	121.62
4	G	401	MSW	OAR-CAU-OAE	-4.32	118.22	124.58
4	B	401	MSW	CAB-OAR-CAU	-3.99	110.95	115.66
4	F	401	MSW	OAT-CAX-CAO	3.91	111.55	106.22
4	C	401	MSW	OAT-CAX-CAO	3.89	111.52	106.22
4	G	401	MSW	CAO-NAQ-CAU	3.88	127.36	121.62
4	B	401	MSW	CAK-CAV-CAX	3.75	128.67	120.63
4	H	401	MSW	OAR-CAU-OAE	-3.74	119.08	124.58
4	E	401	MSW	OAR-CAU-OAE	-3.73	119.10	124.58
4	B	401	MSW	OAT-CAX-CAV	3.67	115.90	109.32
4	C	401	MSW	CAO-CAX-CAV	3.67	117.15	111.36
4	G	401	MSW	OAE-CAU-NAQ	-3.66	119.35	124.96
4	A	401	MSW	OAR-CAU-OAE	-3.61	119.27	124.58
4	A	401	MSW	CAB-OAR-CAU	-3.61	111.41	115.66
4	G	401	MSW	CAJ-CAL-CAV	3.61	125.11	120.65
4	B	401	MSW	OAE-CAU-NAQ	-3.57	119.49	124.96
4	A	401	MSW	CAI-CAK-CAV	3.44	124.90	120.65
4	F	401	MSW	OAT-CAX-CAV	3.31	115.26	109.32
4	D	401	MSW	OAT-CAX-CAV	3.29	115.23	109.32
4	G	401	MSW	CAI-CAK-CAV	3.29	124.71	120.65
4	F	401	MSW	OAE-CAU-NAQ	-3.25	119.98	124.96
4	A	401	MSW	OAT-CAX-CAO	-3.20	101.86	106.22
4	C	401	MSW	OAT-CAX-CAV	3.19	115.04	109.32
4	A	401	MSW	OAE-CAU-NAQ	-3.12	120.18	124.96
4	E	401	MSW	OAE-CAU-NAQ	-3.10	120.21	124.96
4	H	401	MSW	CAO-NAQ-CAU	3.08	126.18	121.62
4	H	401	MSW	CAL-CAV-CAK	3.00	122.04	118.29
4	C	401	MSW	CAK-CAV-CAX	3.00	127.07	120.63
4	H	401	MSW	OAT-CAX-CAV	2.92	114.56	109.32
4	A	401	MSW	CAL-CAV-CAX	2.73	126.49	120.63
4	B	401	MSW	CAJ-CAL-CAV	2.69	123.98	120.65
4	A	401	MSW	CAO-NAQ-CAU	2.61	125.48	121.62
4	H	401	MSW	CAI-CAK-CAV	-2.52	117.53	120.65
4	C	401	MSW	CAI-CAK-CAV	2.52	123.76	120.65
4	C	401	MSW	CAL-CAV-CAK	-2.51	115.16	118.29
4	D	401	MSW	CAO-NAQ-CAU	2.42	125.20	121.62
4	E	401	MSW	CAK-CAV-CAX	2.39	125.76	120.63
4	B	401	MSW	CAO-NAQ-CAU	2.29	125.00	121.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	401	MSW	CAX-CAO-NAQ	2.28	118.36	112.93
4	E	401	MSW	CAL-CAV-CAK	-2.19	115.56	118.29
4	H	401	MSW	OAE-CAU-NAQ	-2.05	121.82	124.96
4	E	401	MSW	CAI-CAK-CAV	2.01	123.14	120.65

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	401	MSW	NAQ-CAO-CAX-OAT
4	C	401	MSW	NAQ-CAO-CAX-CAV
4	C	401	MSW	CAK-CAV-CAX-CAO
4	C	401	MSW	CAL-CAV-CAX-CAO
4	C	401	MSW	NAQ-CAU-OAR-CAB
4	B	401	MSW	NAQ-CAO-CAX-OAT
4	B	401	MSW	NAQ-CAO-CAX-CAV
4	B	401	MSW	CAK-CAV-CAX-CAO
4	B	401	MSW	CAL-CAV-CAX-CAO
4	B	401	MSW	NAQ-CAU-OAR-CAB
4	B	401	MSW	OAE-CAU-OAR-CAB
4	E	401	MSW	CAK-CAV-CAX-CAO
4	E	401	MSW	NAQ-CAU-OAR-CAB
4	E	401	MSW	OAE-CAU-OAR-CAB
4	D	401	MSW	NAQ-CAO-CAX-OAT
4	D	401	MSW	NAQ-CAO-CAX-CAV
4	G	401	MSW	NAQ-CAO-CAX-OAT
4	G	401	MSW	CAK-CAV-CAX-CAO
4	G	401	MSW	CAL-CAV-CAX-CAO
4	G	401	MSW	NAQ-CAU-OAR-CAB
4	G	401	MSW	OAE-CAU-OAR-CAB
4	H	401	MSW	NAQ-CAO-CAX-OAT
4	H	401	MSW	NAQ-CAU-OAR-CAB
4	H	401	MSW	OAE-CAU-OAR-CAB
4	F	401	MSW	NAQ-CAO-CAX-OAT
4	F	401	MSW	NAQ-CAO-CAX-CAV
4	F	401	MSW	NAQ-CAU-OAR-CAB
4	F	401	MSW	OAE-CAU-OAR-CAB
4	A	401	MSW	NAQ-CAO-CAX-OAT
4	A	401	MSW	NAQ-CAO-CAX-CAV
4	A	401	MSW	CAK-CAV-CAX-CAO
4	A	401	MSW	CAL-CAV-CAX-CAO
4	A	401	MSW	NAQ-CAU-OAR-CAB

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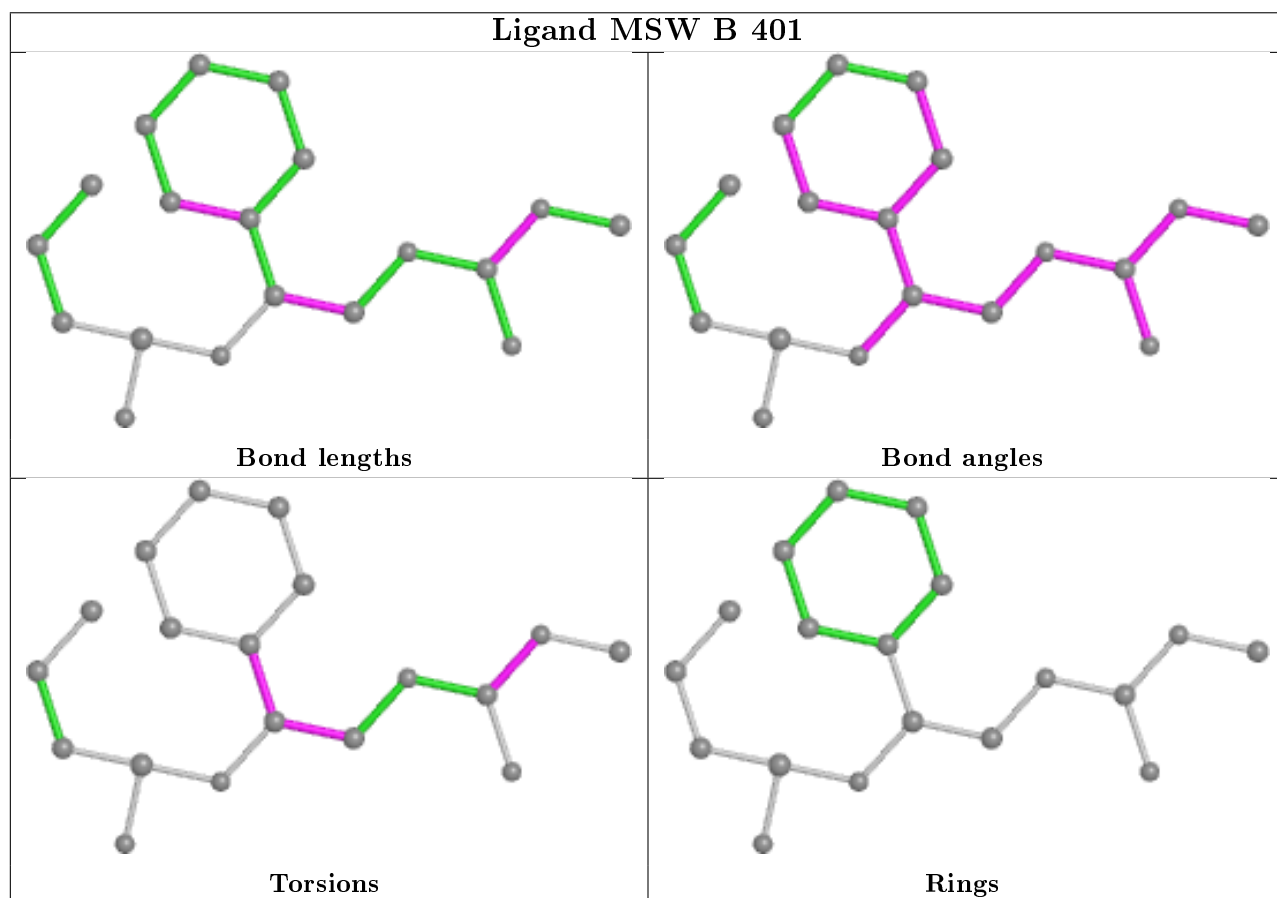
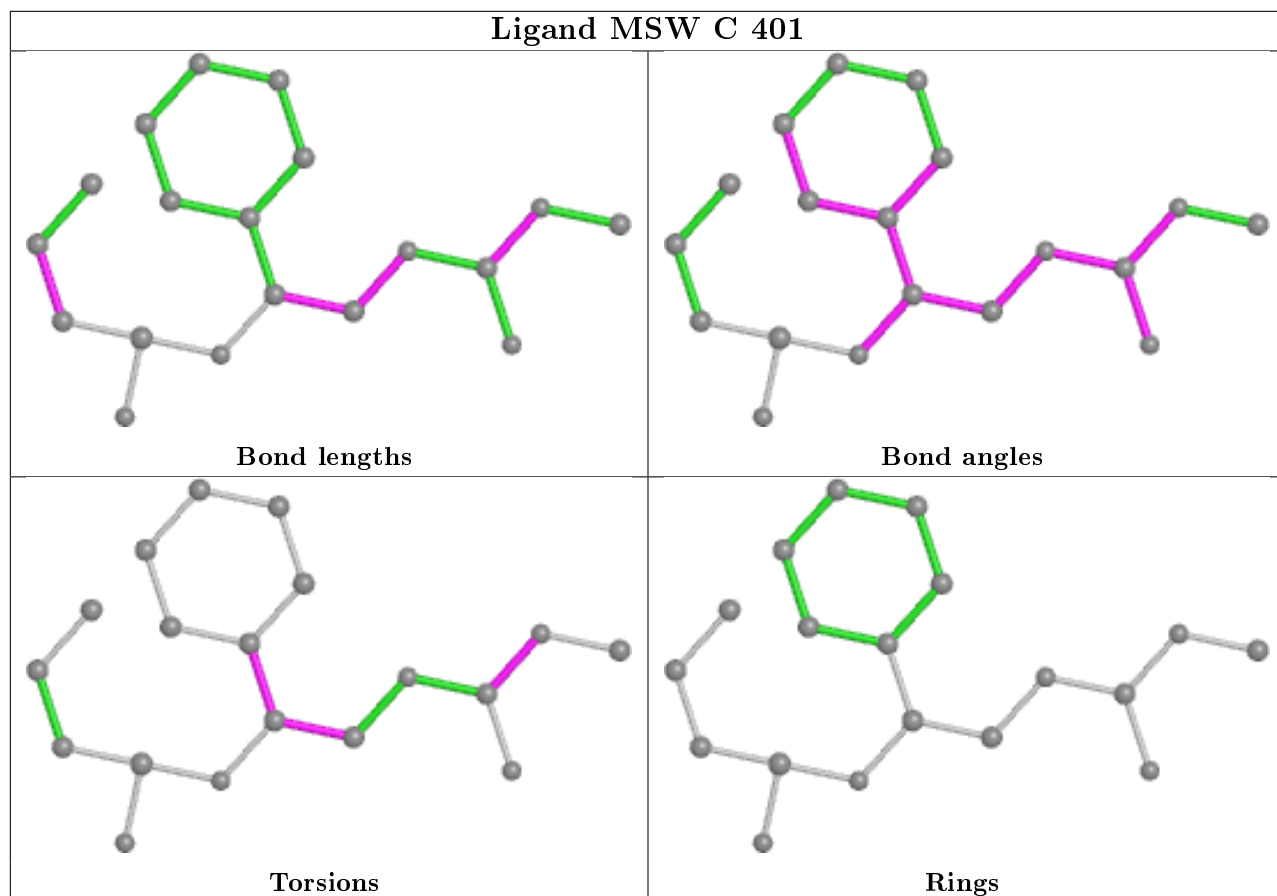
Mol	Chain	Res	Type	Atoms
4	A	401	MSW	OAE-CAU-OAR-CAB
4	C	401	MSW	OAE-CAU-OAR-CAB
4	E	401	MSW	CAL-CAV-CAX-CAO
4	G	401	MSW	NAQ-CAO-CAX-CAV
4	A	401	MSW	CAA-CAM-CAN-PAY
4	D	401	MSW	NAQ-CAU-OAR-CAB
4	D	401	MSW	OAE-CAU-OAR-CAB
4	G	401	MSW	CAX-CAO-NAQ-CAU
4	H	401	MSW	NAQ-CAO-CAX-CAV

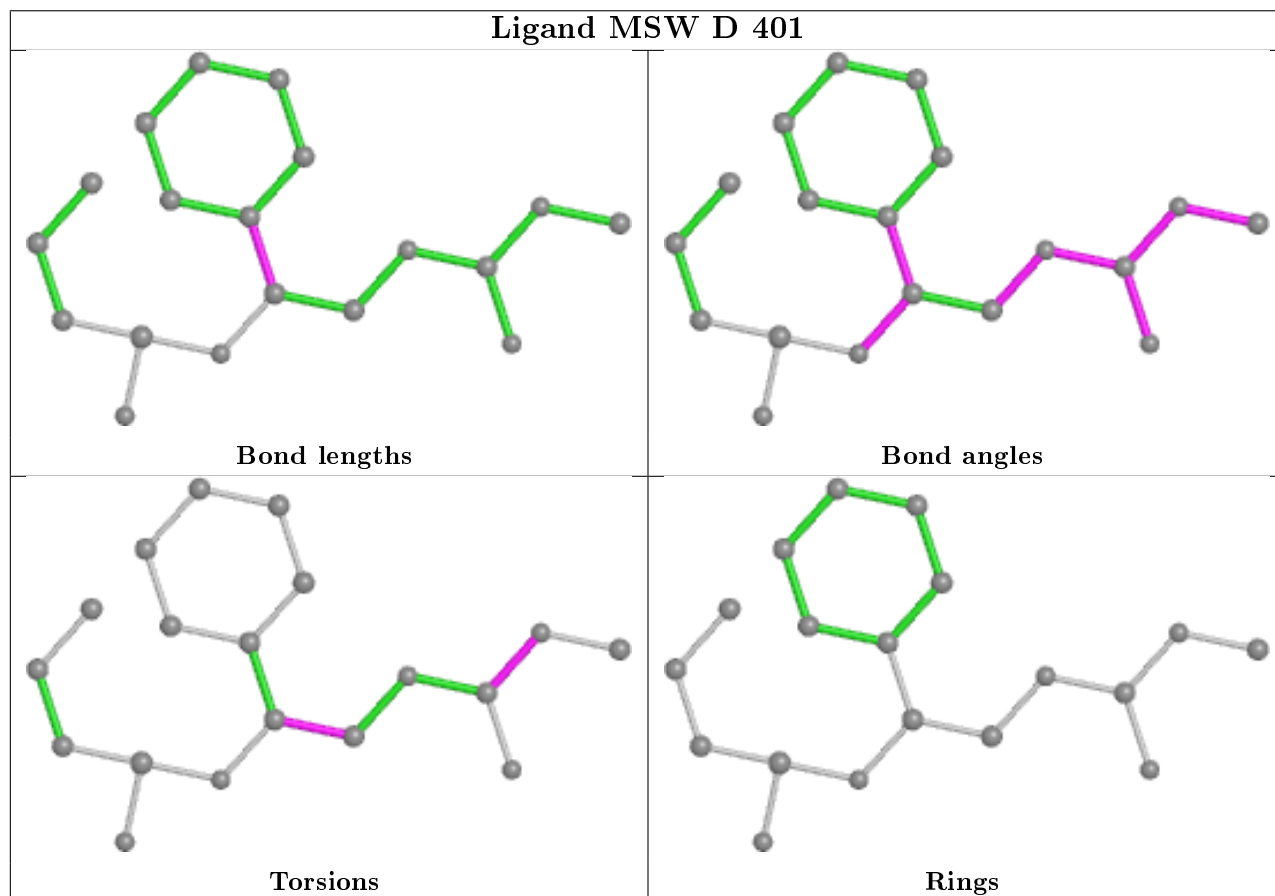
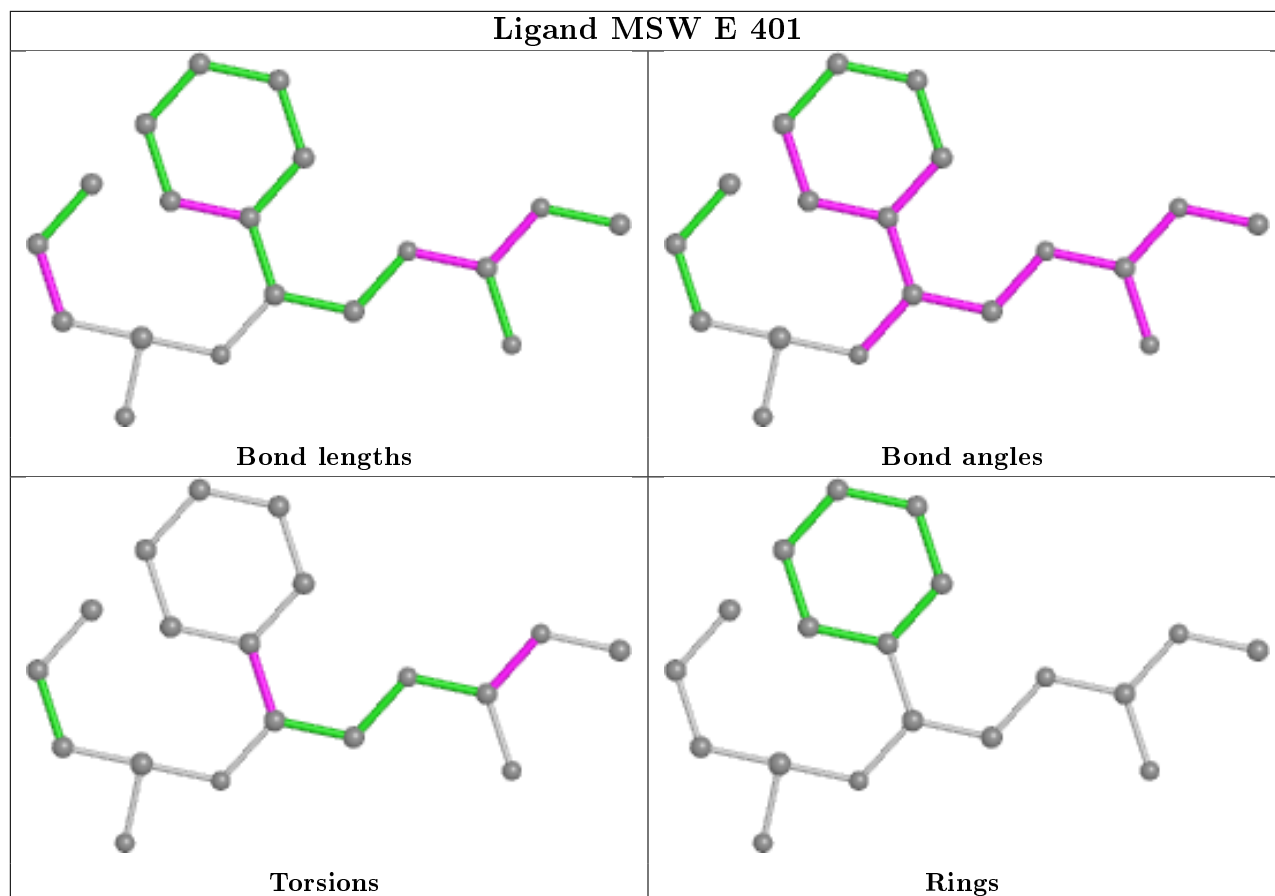
There are no ring outliers.

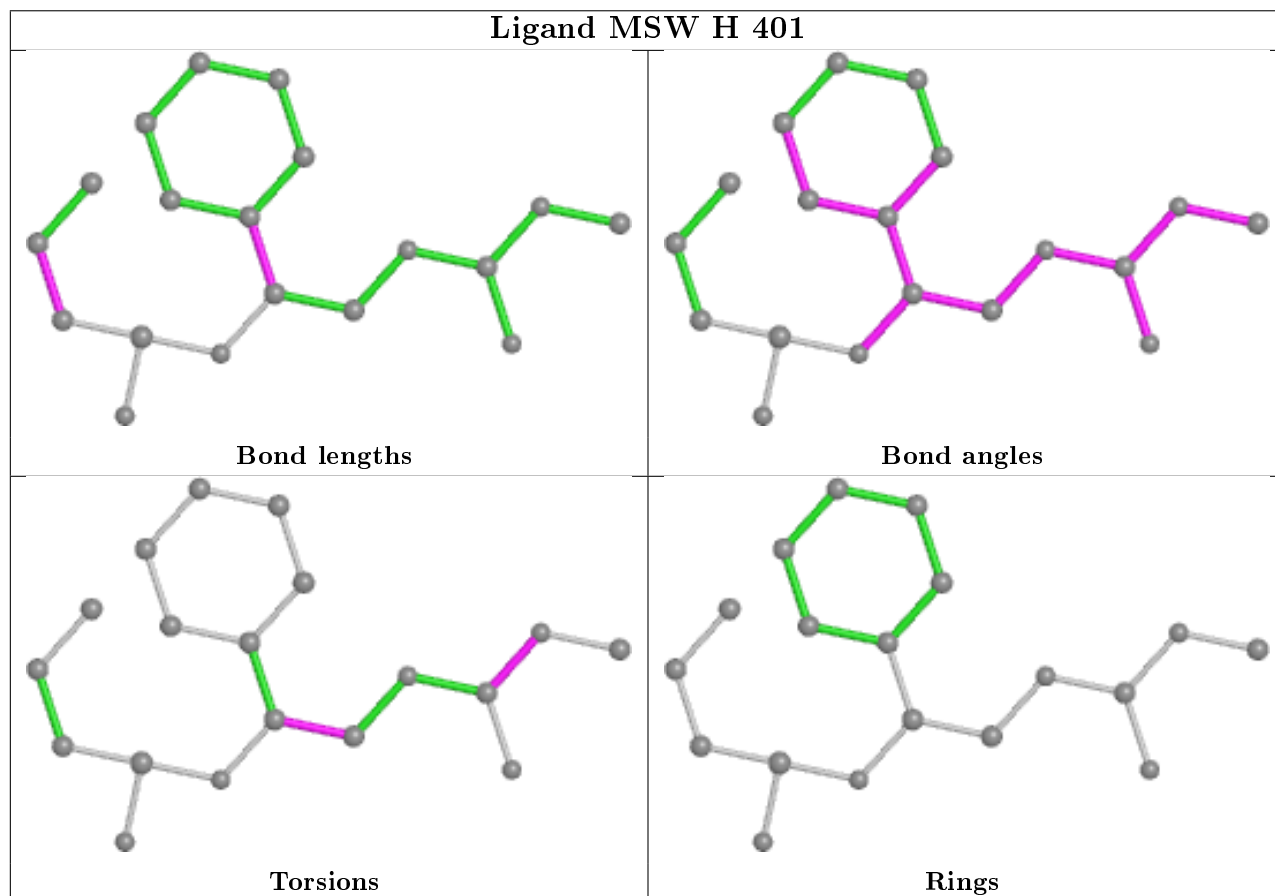
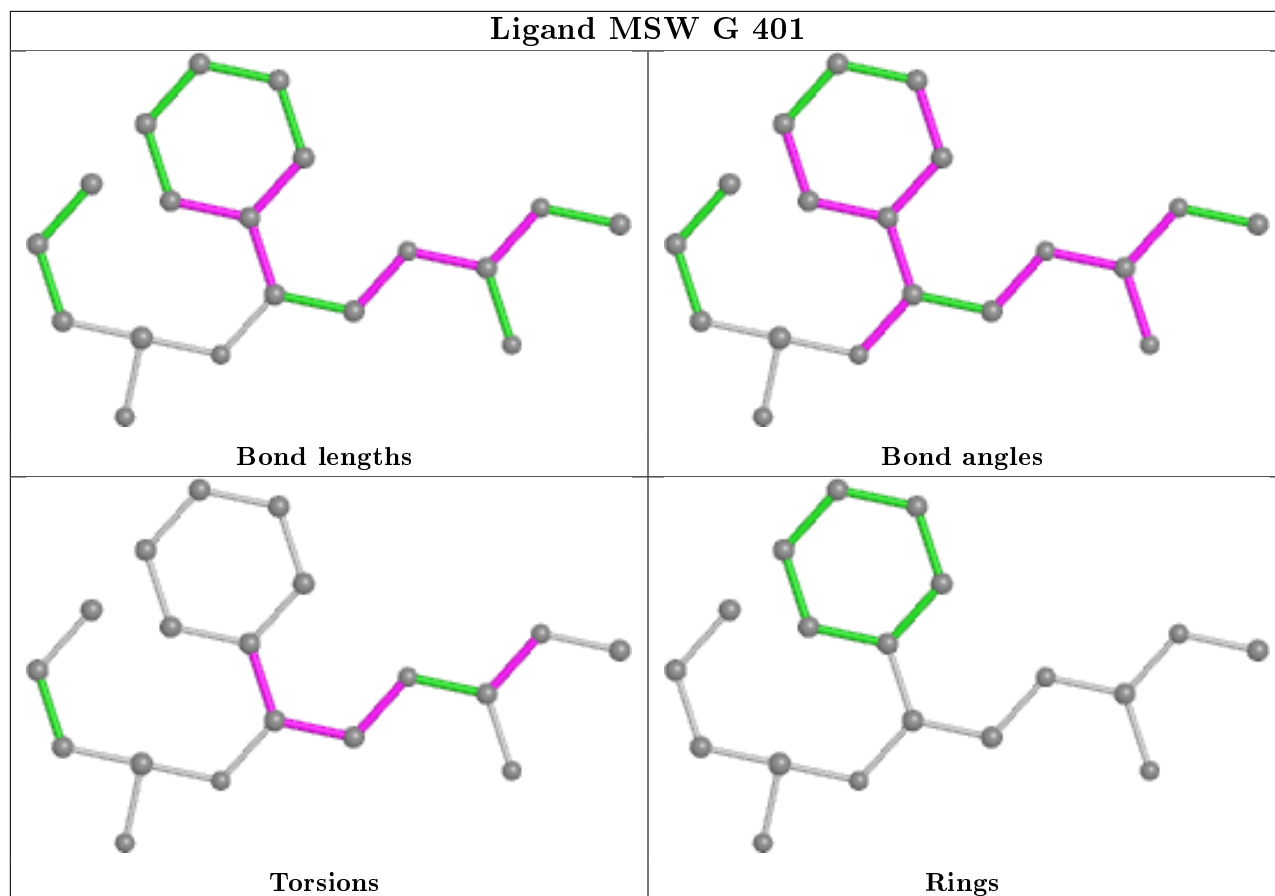
7 monomers are involved in 22 short contacts:

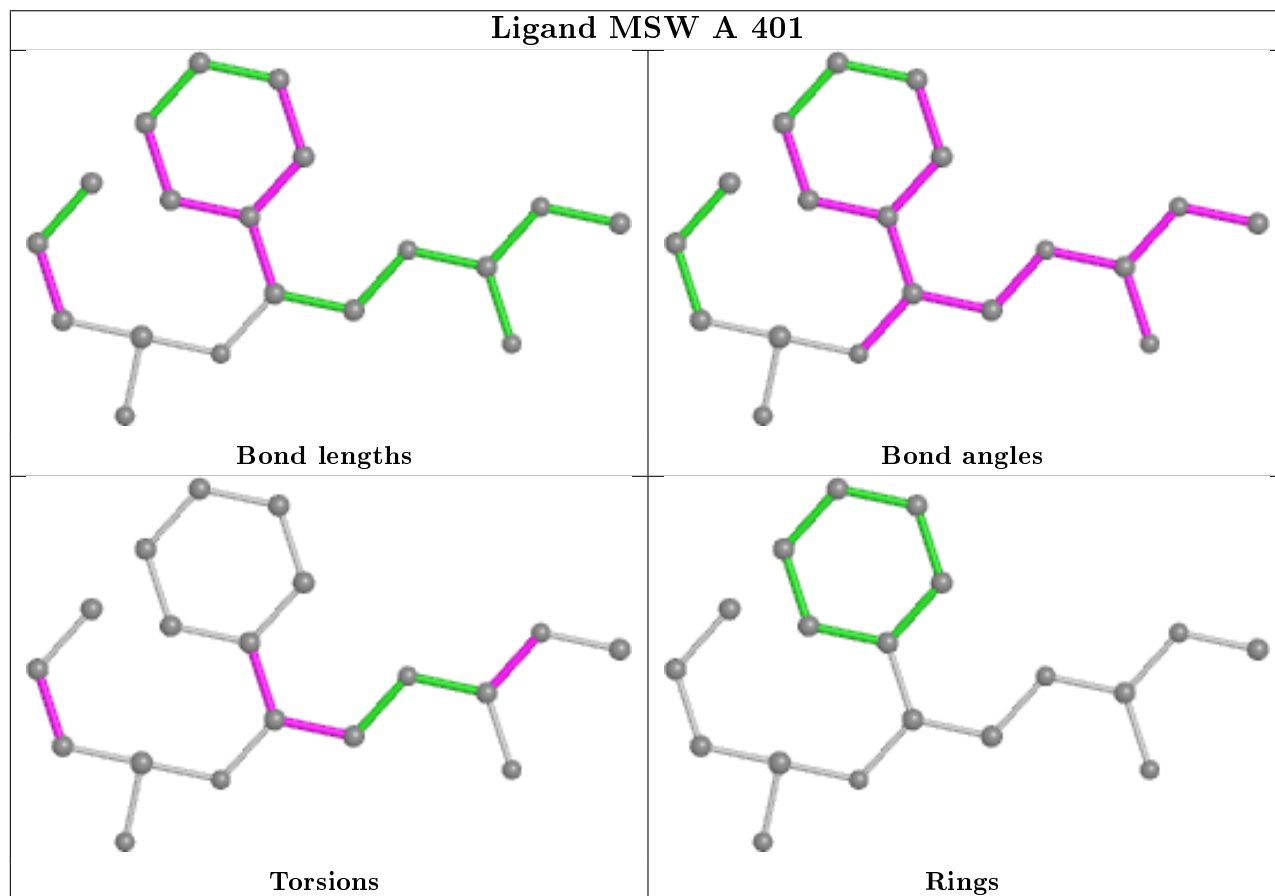
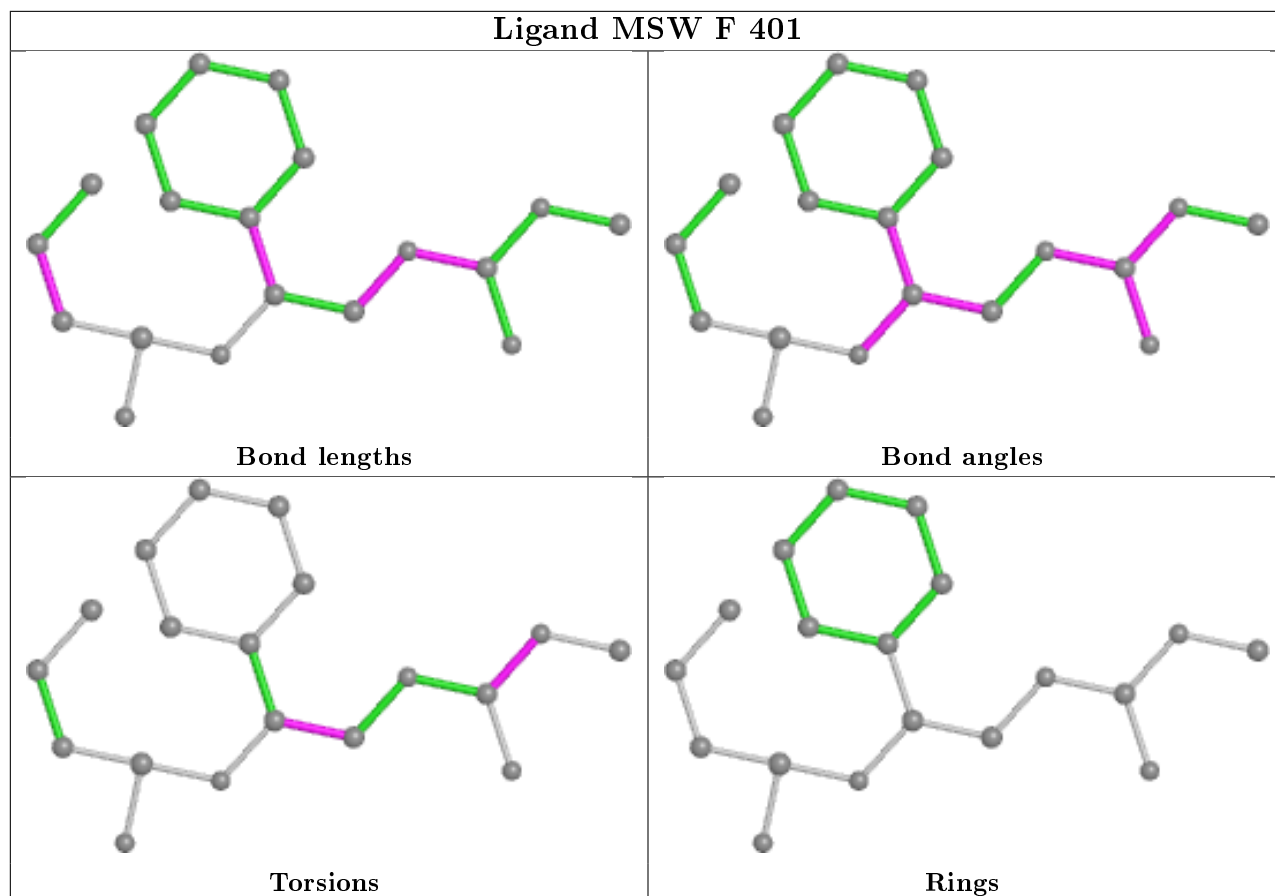
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	401	MSW	4	0
4	B	401	MSW	6	0
4	D	401	MSW	2	0
4	G	401	MSW	2	0
4	H	401	MSW	4	0
4	F	401	MSW	1	0
4	A	401	MSW	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	317/317 (100%)	-0.61	1 (0%) 94 94	16, 26, 44, 76	0
1	B	317/317 (100%)	-0.47	2 (0%) 89 89	19, 34, 56, 86	0
1	C	316/317 (99%)	-0.42	2 (0%) 89 89	19, 30, 53, 83	0
1	D	309/317 (97%)	-0.36	4 (1%) 77 77	20, 31, 60, 93	0
1	E	314/317 (99%)	-0.38	2 (0%) 89 89	16, 29, 55, 105	0
1	F	317/317 (100%)	-0.33	1 (0%) 94 94	23, 37, 58, 81	0
1	G	317/317 (100%)	-0.36	2 (0%) 89 89	24, 39, 59, 77	0
1	H	317/317 (100%)	-0.29	4 (1%) 77 77	24, 39, 62, 101	0
All	All	2524/2536 (99%)	-0.40	18 (0%) 87 87	16, 33, 58, 105	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	317	PRO	5.0
1	D	317	PRO	4.4
1	H	317	PRO	4.1
1	B	317	PRO	3.8
1	H	311	CYS	3.1
1	H	3	SER	3.0
1	C	146	ALA	3.0
1	G	24	GLY	2.9
1	G	317	PRO	2.9
1	D	306	VAL	2.7
1	E	317	PRO	2.6
1	D	316	THR	2.6
1	H	24	GLY	2.3
1	A	317	PRO	2.3
1	F	5	SER	2.3
1	D	314	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	107	GLY	2.1
1	B	96	ASN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	P	2	14/15	0.73	0.61	75,120,134,140	0
3	NAG	N	2	14/15	0.75	0.50	81,98,107,110	0
3	NAG	O	2	14/15	0.76	0.40	74,98,104,109	0
2	NAG	I	3	14/15	0.78	0.33	75,85,88,90	0
3	NAG	M	2	14/15	0.79	0.42	63,72,78,79	0
2	NAG	K	4	14/15	0.79	0.47	75,86,97,100	0
2	NAG	I	4	14/15	0.80	0.38	69,84,93,97	0
2	NAG	K	3	14/15	0.82	0.40	66,84,100,110	0
3	NAG	O	1	14/15	0.84	0.24	65,79,93,103	0
3	NAG	L	2	14/15	0.85	0.51	74,81,86,86	0
3	NAG	J	2	14/15	0.86	0.39	58,73,82,83	0
3	NAG	P	1	14/15	0.87	0.37	66,81,98,103	0
3	NAG	N	1	14/15	0.91	0.31	50,63,71,81	0
3	NAG	M	1	14/15	0.91	0.32	54,57,65,71	0
2	NAG	I	2	14/15	0.93	0.23	40,47,60,72	0
2	NAG	K	2	14/15	0.93	0.24	39,51,58,65	0
2	NAG	I	1	14/15	0.94	0.15	38,42,46,47	0
3	NAG	J	1	14/15	0.95	0.24	48,53,58,67	0
3	NAG	L	1	14/15	0.95	0.26	47,55,61,70	0
2	NAG	K	1	14/15	0.96	0.13	32,37,41,41	0

## 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

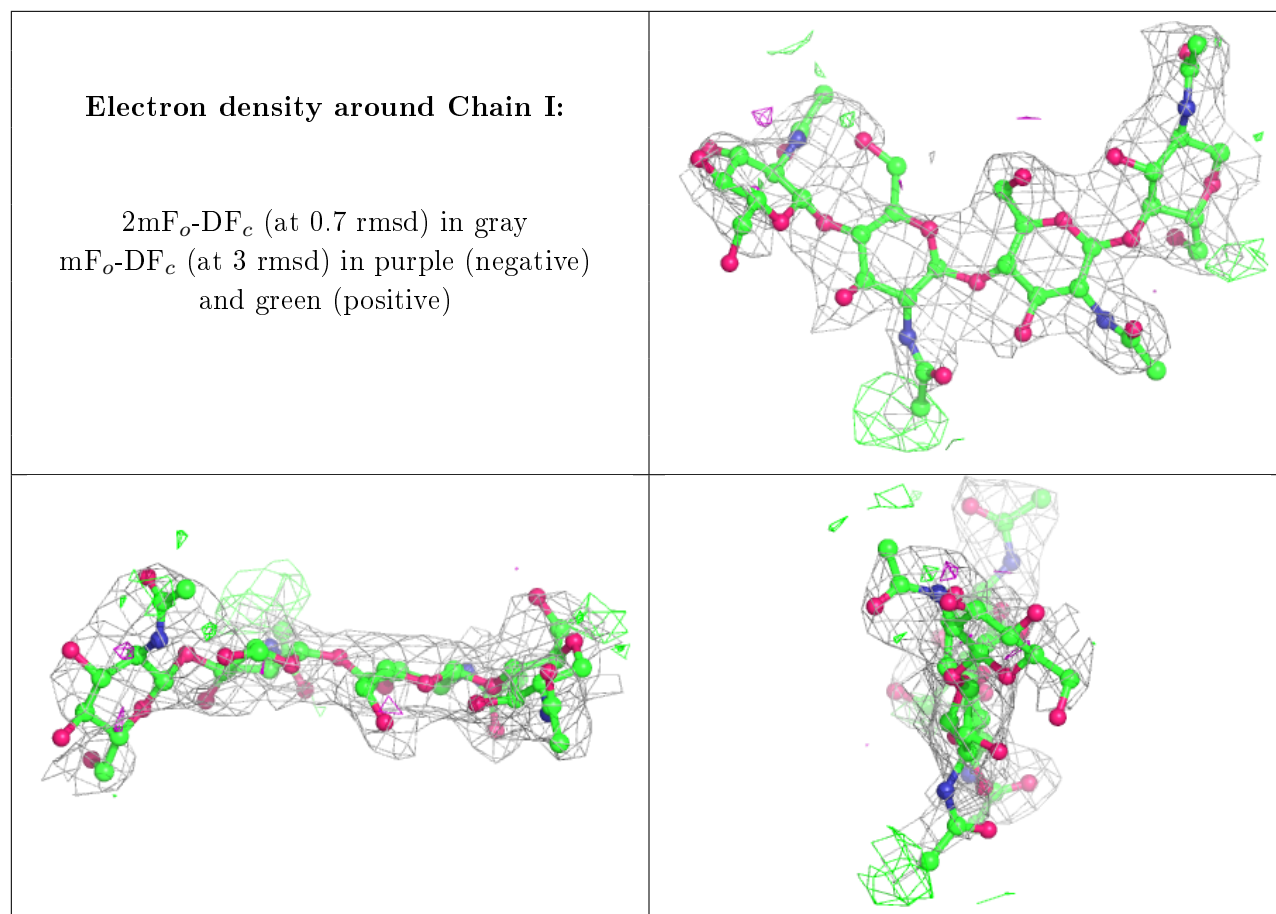
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	P	2	14/15	0.73	0.61	75,120,134,140	0

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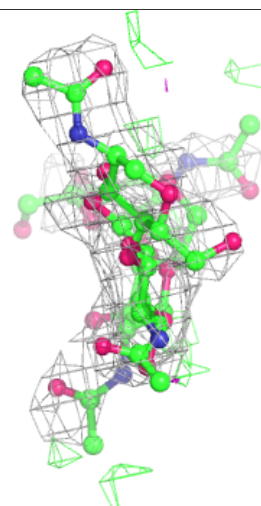
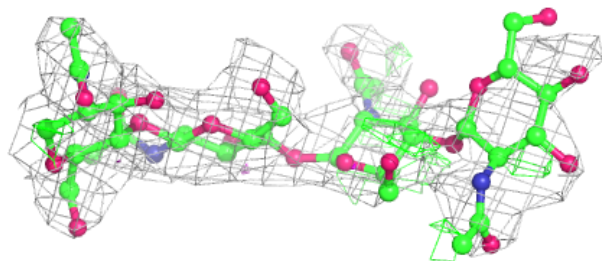
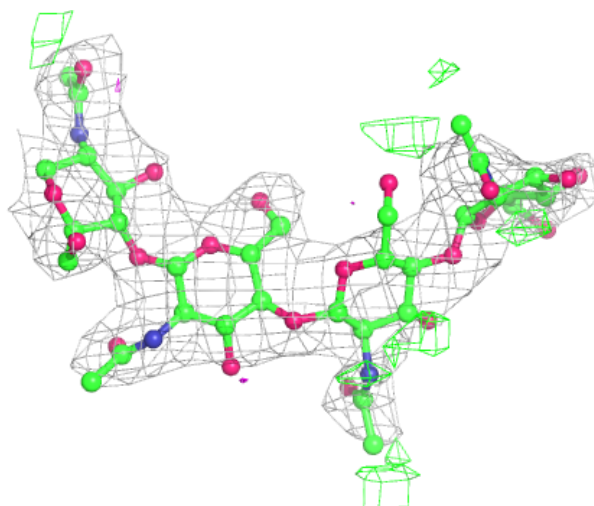
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	N	2	14/15	0.75	0.50	81,98,107,110	0
3	NAG	O	2	14/15	0.76	0.40	74,98,104,109	0
2	NAG	I	3	14/15	0.78	0.33	75,85,88,90	0
2	NAG	K	4	14/15	0.79	0.47	75,86,97,100	0
3	NAG	M	2	14/15	0.79	0.42	63,72,78,79	0
2	NAG	I	4	14/15	0.80	0.38	69,84,93,97	0
2	NAG	K	3	14/15	0.82	0.40	66,84,100,110	0
3	NAG	O	1	14/15	0.84	0.24	65,79,93,103	0
3	NAG	L	2	14/15	0.85	0.51	74,81,86,86	0
3	NAG	J	2	14/15	0.86	0.39	58,73,82,83	0
3	NAG	P	1	14/15	0.87	0.37	66,81,98,103	0
3	NAG	N	1	14/15	0.91	0.31	50,63,71,81	0
3	NAG	M	1	14/15	0.91	0.32	54,57,65,71	0
2	NAG	K	2	14/15	0.93	0.24	39,51,58,65	0
2	NAG	I	2	14/15	0.93	0.23	40,47,60,72	0
2	NAG	I	1	14/15	0.94	0.15	38,42,46,47	0
3	NAG	J	1	14/15	0.95	0.24	48,53,58,67	0
3	NAG	L	1	14/15	0.95	0.26	47,55,61,70	0
2	NAG	K	1	14/15	0.96	0.13	32,37,41,41	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



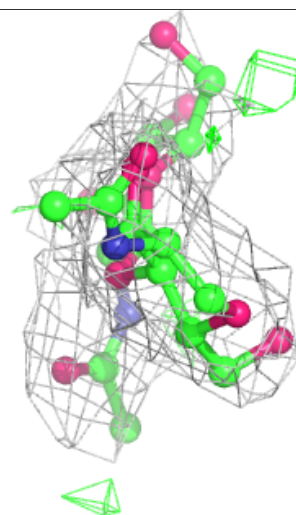
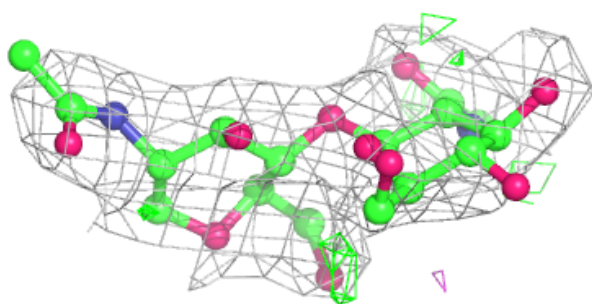
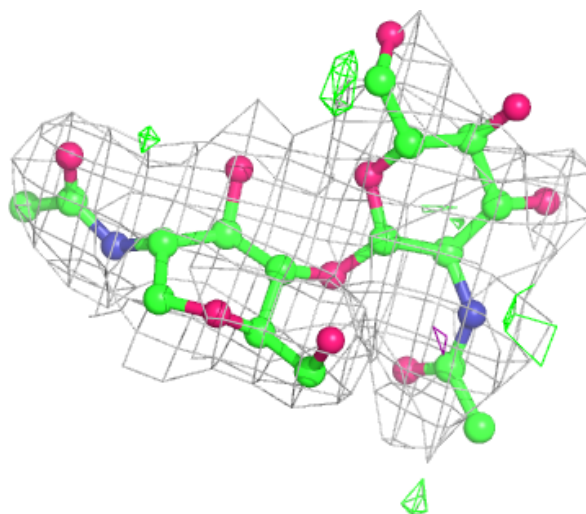
**Electron density around Chain K:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



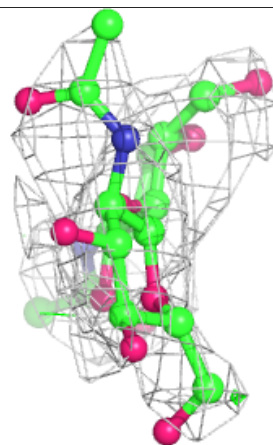
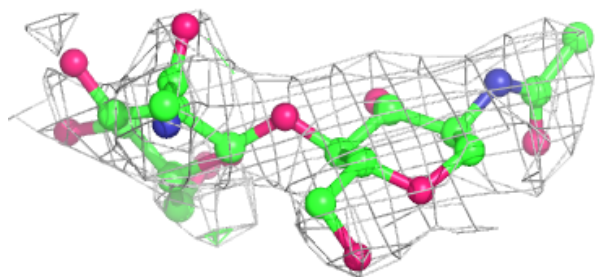
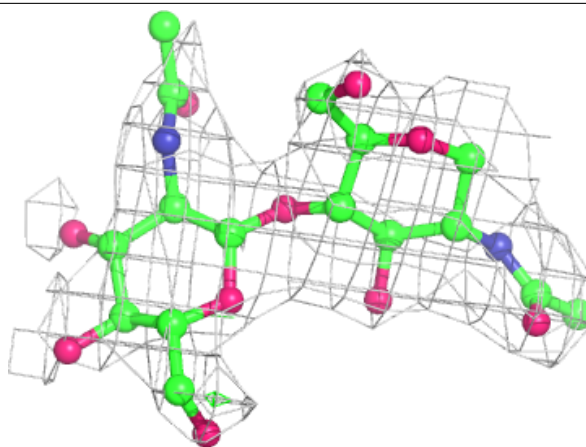
**Electron density around Chain J:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain L:**

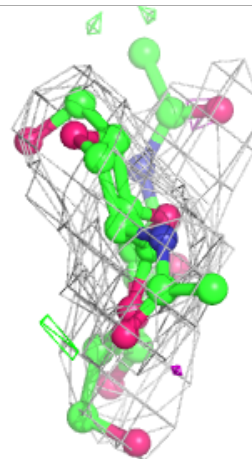
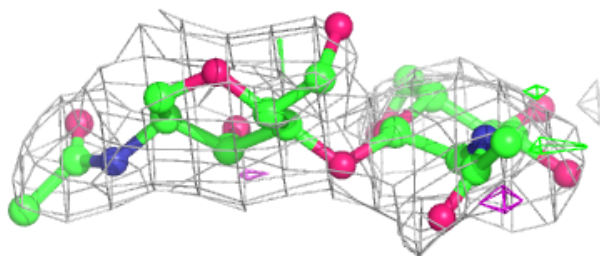
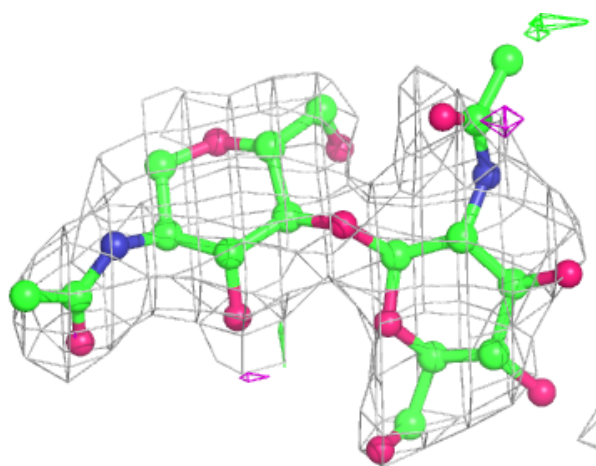
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





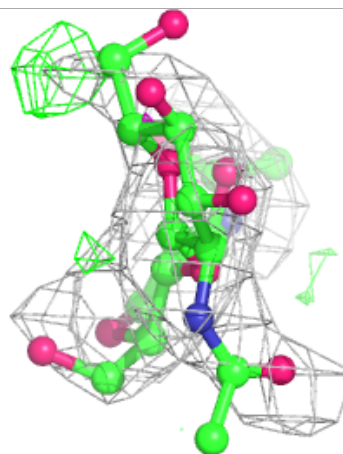
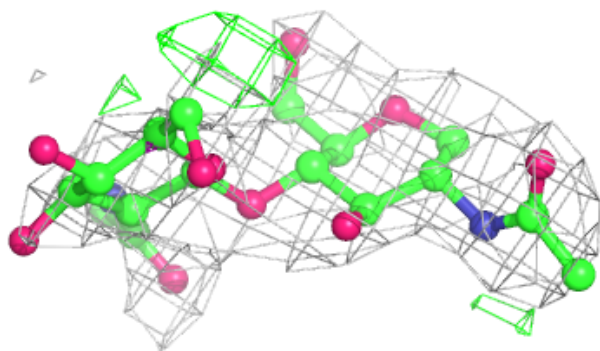
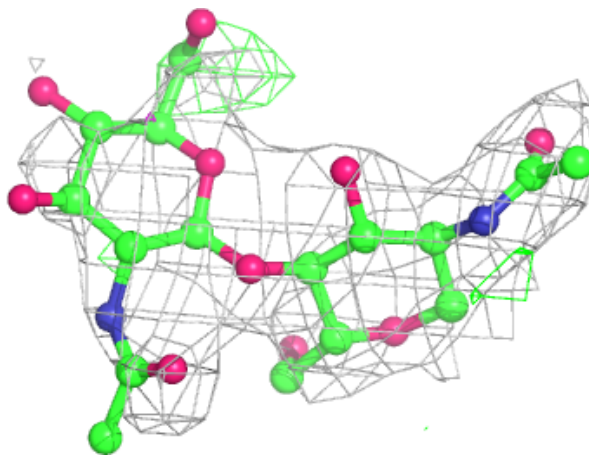
**Electron density around Chain M:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



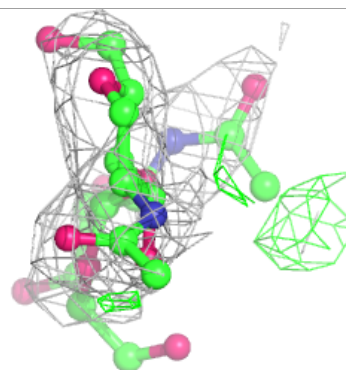
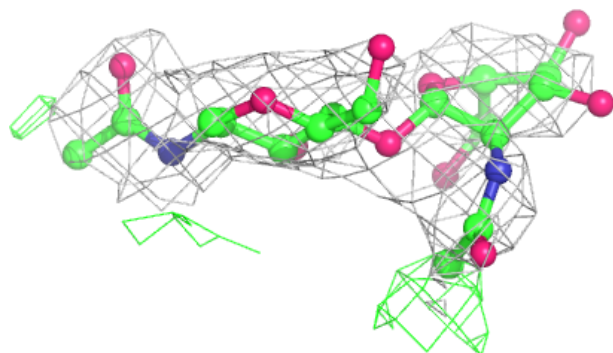
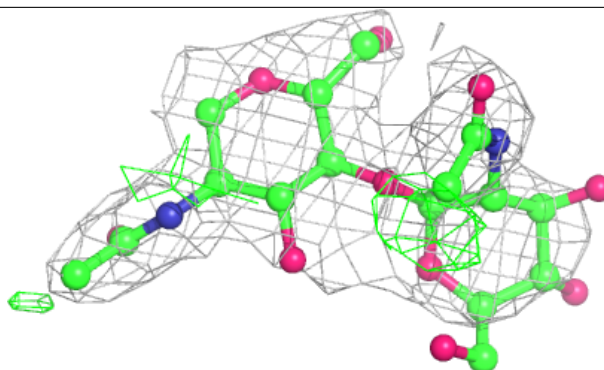
**Electron density around Chain N:**

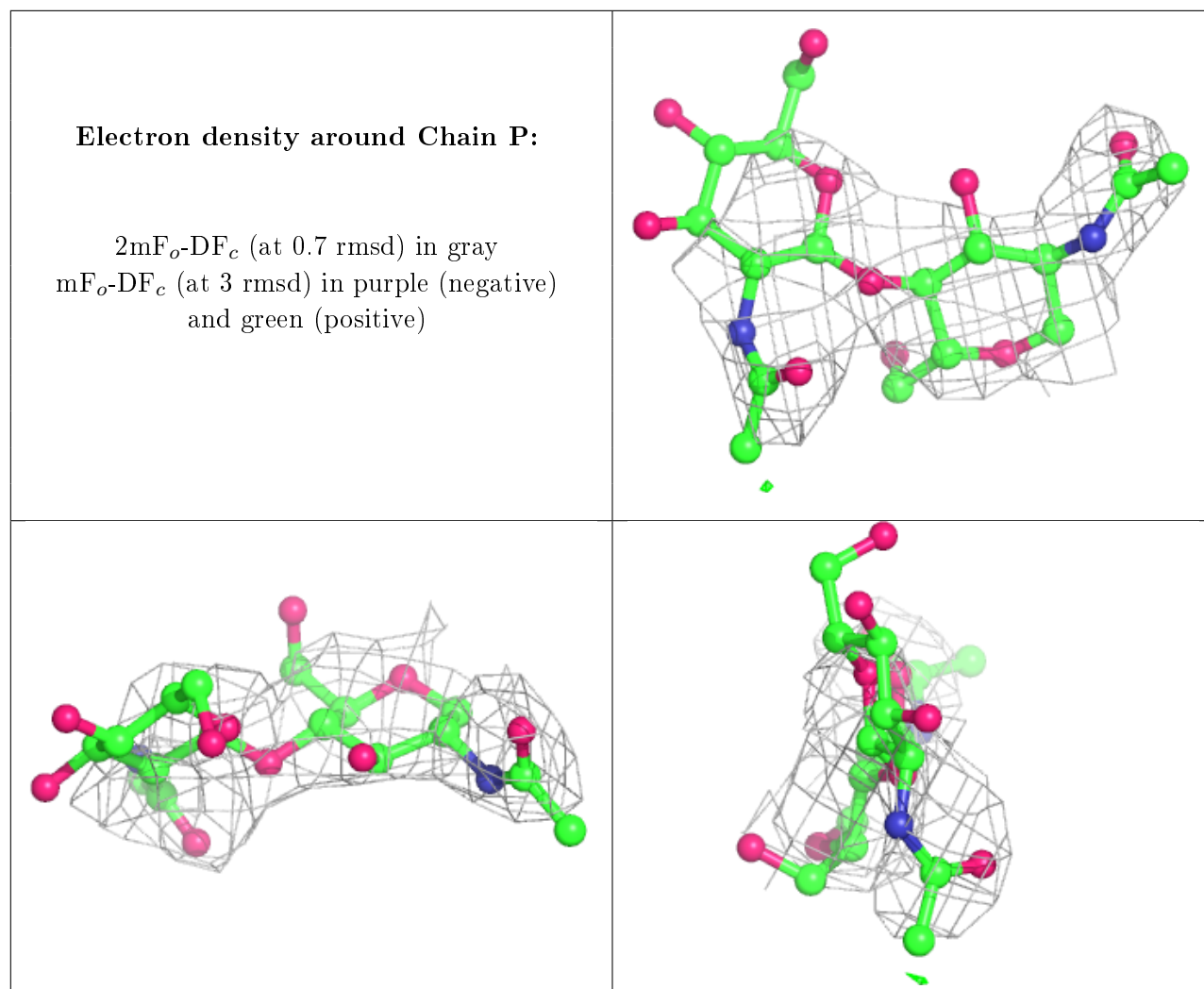
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain O:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



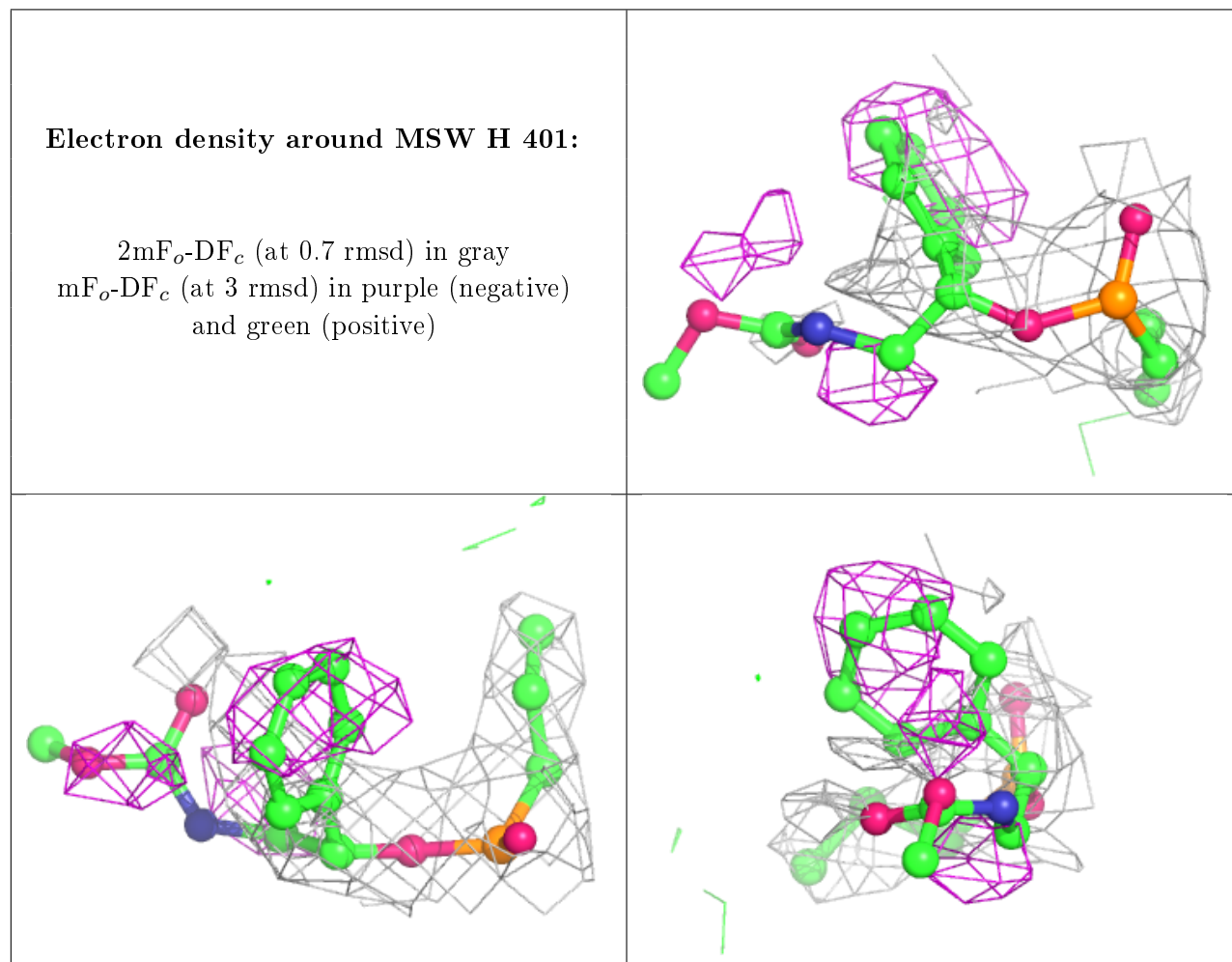


## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

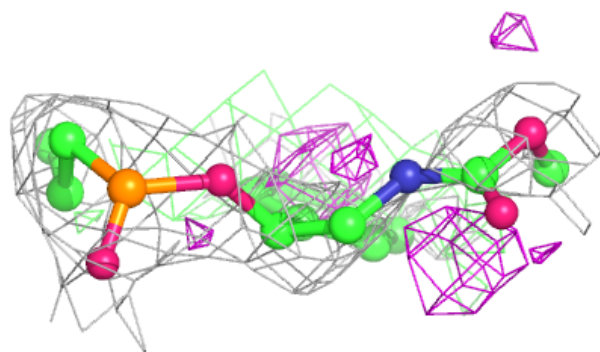
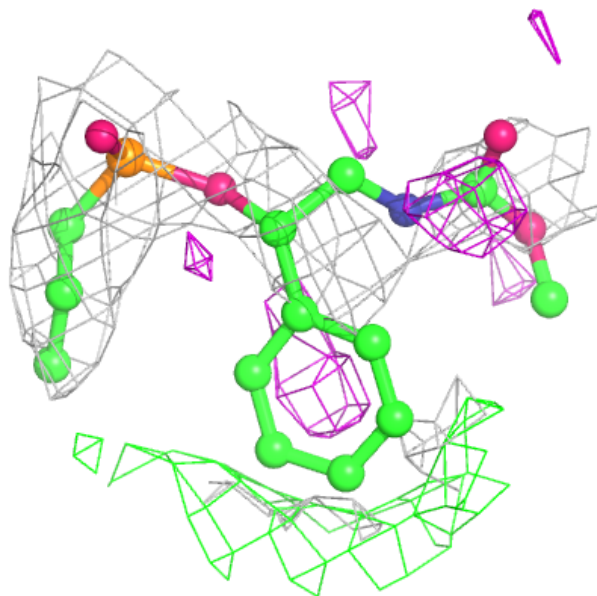
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	MSW	H	401	19/20	0.85	0.41	48,115,146,152	0
4	MSW	A	401	19/20	0.87	0.32	38,101,113,115	0
4	MSW	B	401	19/20	0.91	0.28	42,78,108,123	0
4	MSW	G	401	19/20	0.91	0.27	49,84,101,110	0
4	MSW	C	401	19/20	0.95	0.21	35,60,71,84	0
4	MSW	E	401	19/20	0.95	0.21	32,67,79,80	0
4	MSW	D	401	19/20	0.95	0.18	32,46,56,59	0
4	MSW	F	401	19/20	0.97	0.18	40,46,48,54	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



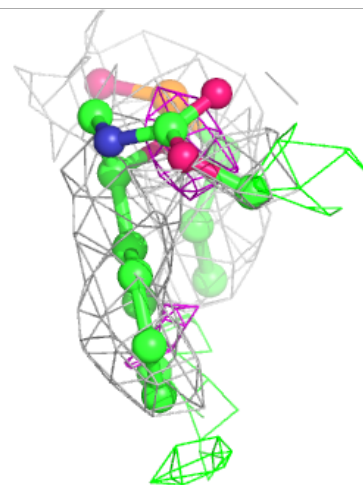
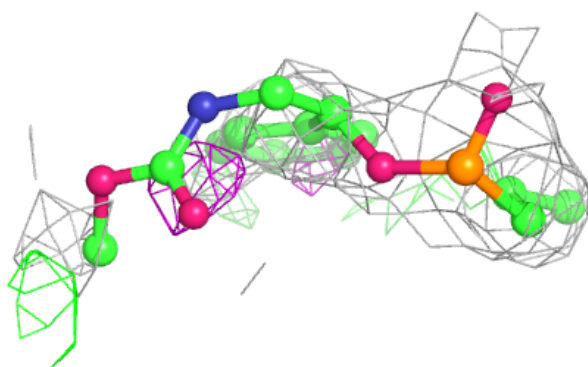
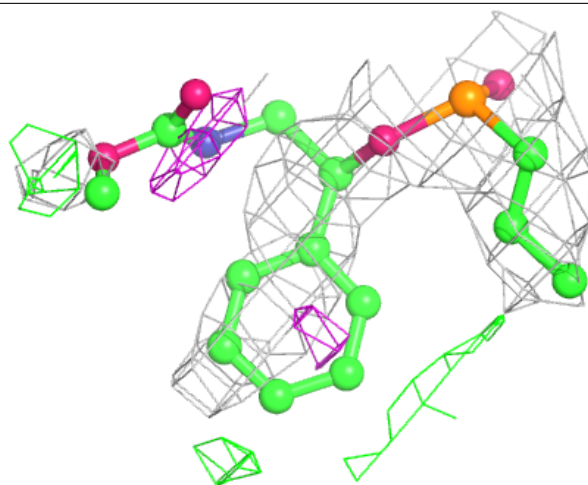
**Electron density around MSW A 401:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around MSW B 401:**

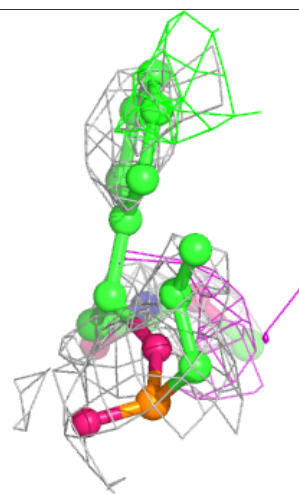
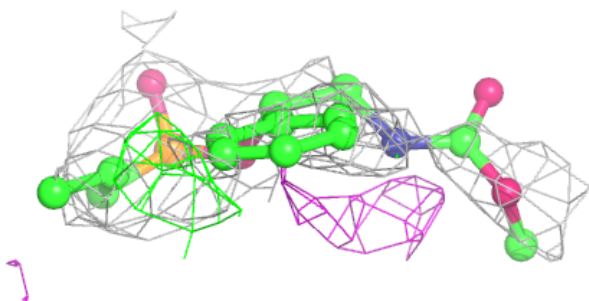
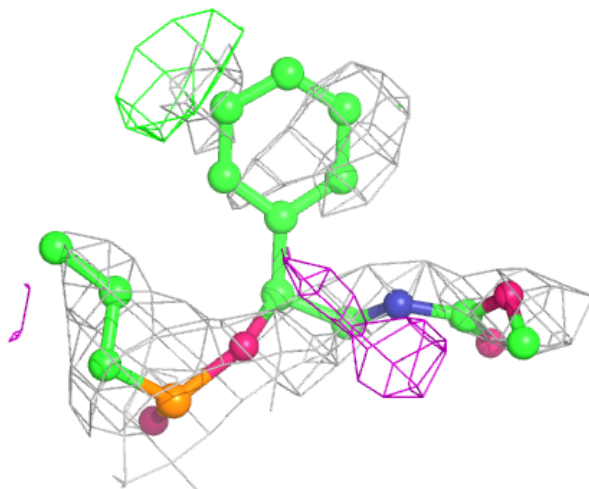
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



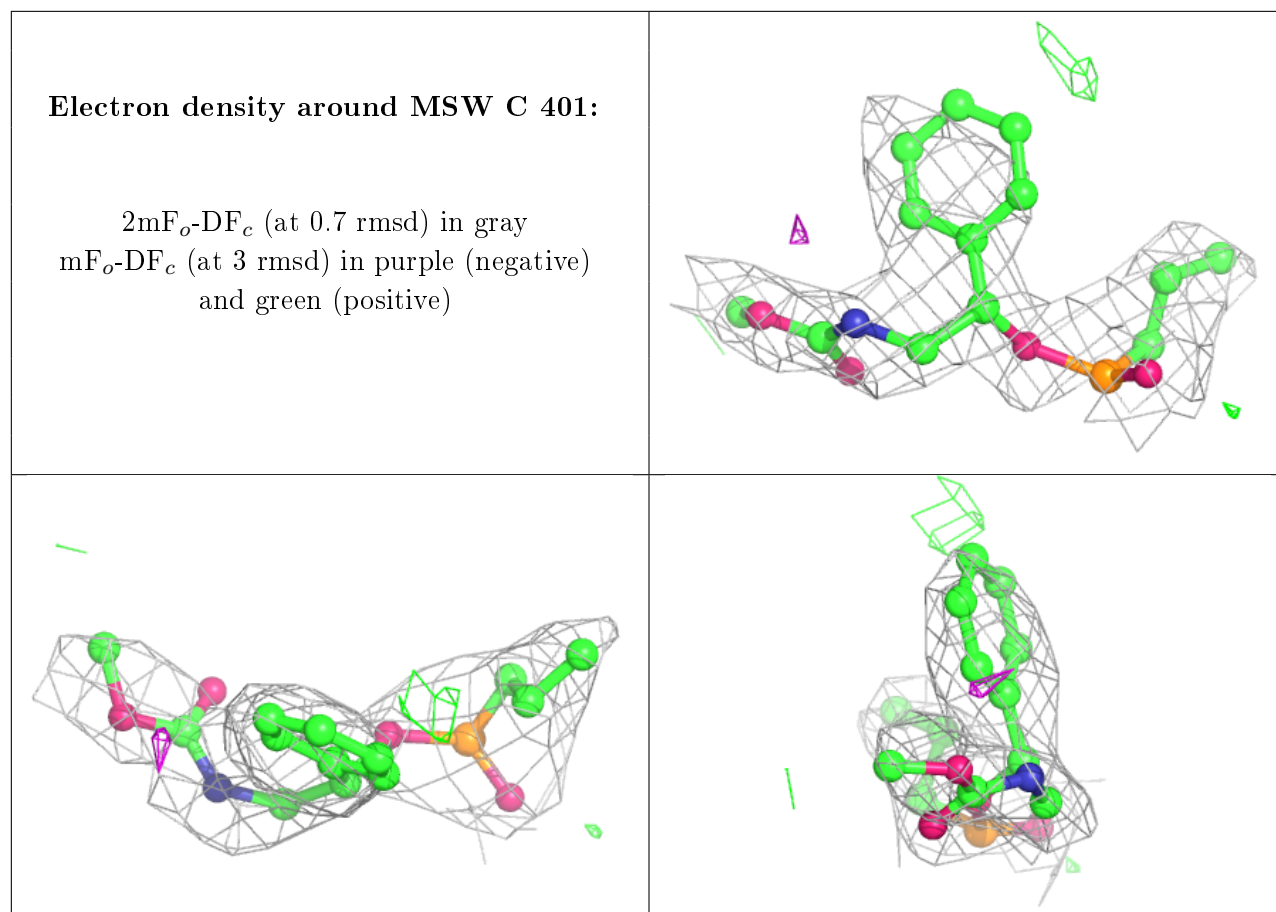


**Electron density around MSW G 401:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

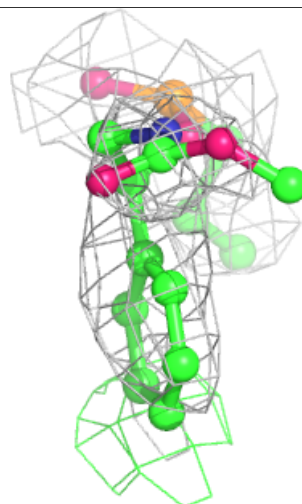
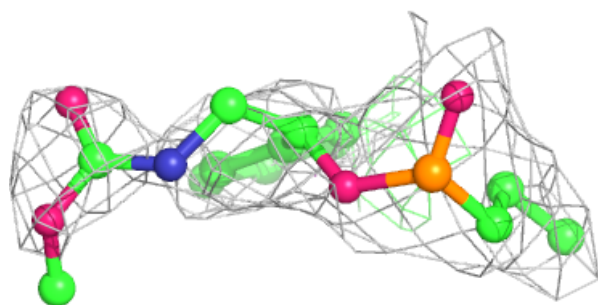
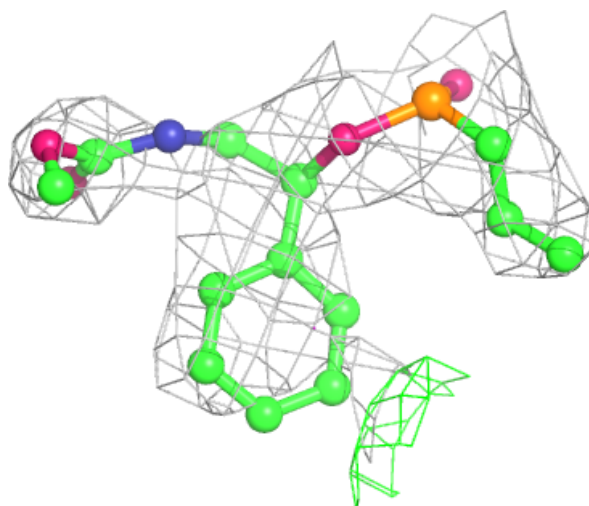






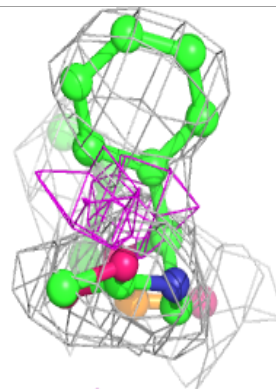
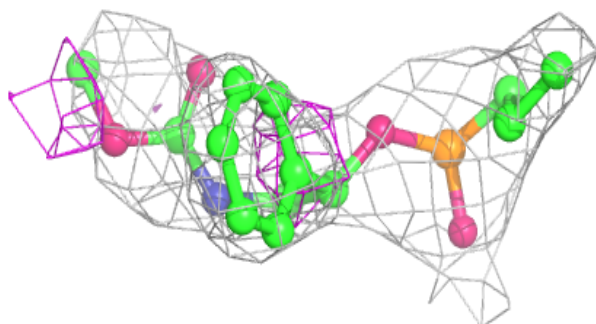
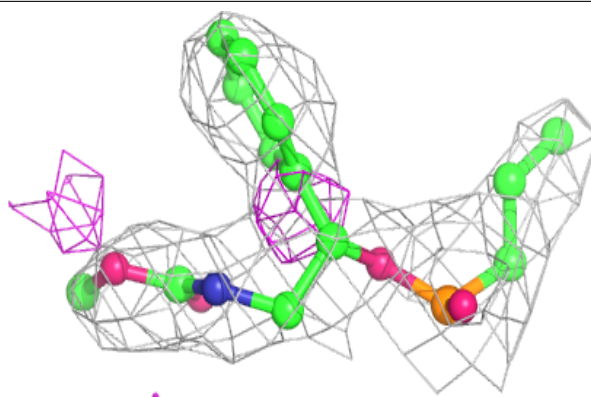
**Electron density around MSW E 401:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

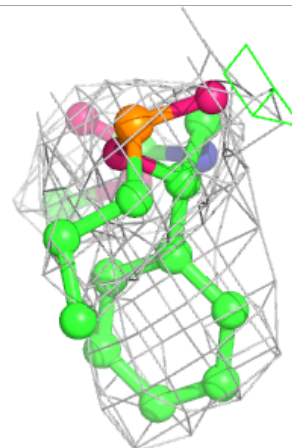
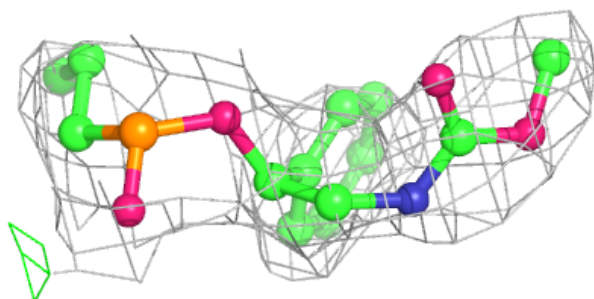
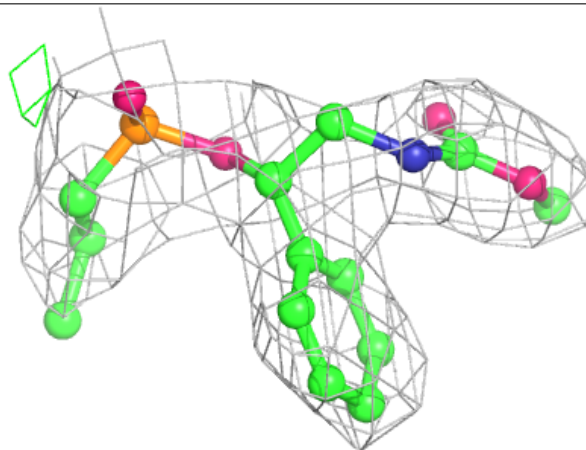


**Electron density around MSW D 401:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around MSW F 401:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers

There are no such residues in this entry.